09/898,941



| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 1.26 | 1.26 |

FILE 'REGISTRY' ENTERED AT 16:56:59 ON 09 NOV 2005


Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 7 NOV 2005 HIGHEST RN 866913-62-4
DICTIONARY FILE UPDATES: 7 NOV 2005 HIGHEST RN 866913-62-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

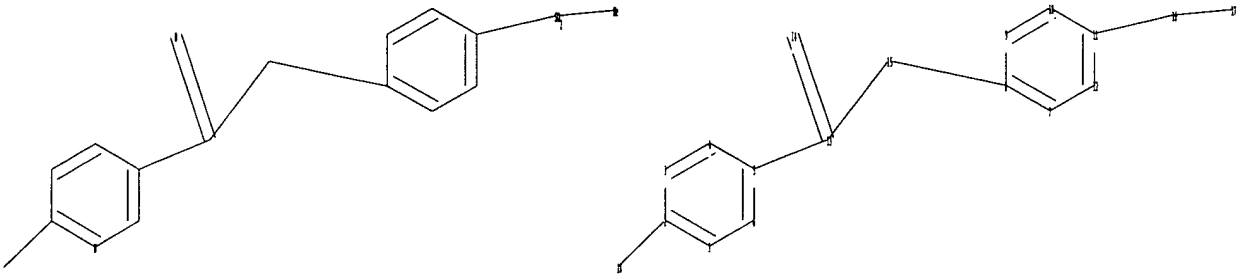
**********
* *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
* *
**********

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\rkc941.str



```
chain nodes :
13  14  15  16  17  18
ring nodes :
1  2  3  4  5  6  7  8  9  10  11  12
chain bonds :
2-18  5-13  8-15  11-16  13-14  13-15  16-17
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  7-8  7-12  8-9  9-10  10-11  11-12
exact/norm bonds :
13-14
exact bonds :
2-18  5-13  8-15  11-16  13-15  16-17
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6  7-8  7-12  8-9  9-10  10-11  11-12
isolated ring systems :
containing 1 : 7 :


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:Atom  13:CLASS  14:CLASS  15:CLASS  16:CLASS  17:CLASS  18:CLASS



L1      STRUCTURE UPLOADED

=> s k1 ful
L2       19574 K1

=> d 1 fhitstr
'FHITSTR' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual
fields or predefined formats.  The predefined substance formats
are:  (RN = CAS Registry Number)

REG     - RN
SAM     - Index Name, MF, and structure - no RN
FIDE    - All substance data, except sequence data
IDE     - FIDE, but only 50 names
SQIDE   - IDE, plus sequence data
SQIDE3  - Same as SQIDE, but 3-letter amino acid codes are used
SQD     - Protein sequence data, includes RN
SQD3    - Same as SQD, but 3-letter amino acid codes are used
SQN     - Protein sequence name information, includes RN

CALC    - Table of calculated properties
EPROP   - Table of experimental properties
PROP    - EPROP and CALC

Any CA File format may be combined with any substance format to
obtain CA references citing the substance.  The substance formats
must be cited first.  The CA File predefined formats are:

ABS  -- Abstract
APPS -- Application and Priority Information
BIB  -- CA Accession Number, plus Bibliographic Data
```

```
CAN  -- CA Accession Number
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)
IND  -- Index Data
IPC  -- International Patent Classification
PATS -- PI, SO
STD  -- BIB, IPC, and NCL

IABS -- ABS, indented, with text labels
IBIB -- BIB, indented, with text labels
ISTD -- STD format, indented

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when
it is available.
The MAX format is the same as ALL.
The IALL format is the same as ALL with BIB ABS and IND indented,
with text labels.

For additional information, please consult the following help
messages:

HELP DFIELDS -- To see a complete list of individual display fields.
HELP FORMATS -- To see detailed descriptions of the predefined formats.
ENTER DISPLAY FORMAT (IDE):d 1
'D' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual
fields or predefined formats.  The predefined substance formats
are:  (RN = CAS Registry Number)

REG    - RN
SAM    - Index Name, MF, and structure - no RN
FIDE   - All substance data, except sequence data
IDE    - FIDE, but only 50 names
SQIDE  - IDE, plus sequence data
SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used
SQD    - Protein sequence data, includes RN
SQD3   - Same as SQD, but 3-letter amino acid codes are used
SQN    - Protein sequence name information, includes RN

CALC   - Table of calculated properties
EPROP  - Table of experimental properties
PROP   - EPROP and CALC

Any CA File format may be combined with any substance format to
obtain CA references citing the substance.  The substance formats
must be cited first.  The CA File predefined formats are:

ABS  -- Abstract
APPS -- Application and Priority Information
BIB  -- CA Accession Number, plus Bibliographic Data
CAN  -- CA Accession Number
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)
```

```
IND  -- Index Data
IPC  -- International Patent Classification
PATS -- PI, SO
STD  -- BIB, IPC, and NCL

IABS -- ABS, indented, with text labels
IBIB -- BIB, indented, with text labels
ISTD -- STD format, indented

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when
it is available.
The MAX format is the same as ALL.
The IALL format is the same as ALL with BIB ABS and IND indented,
with text labels.

For additional information, please consult the following help
messages:

HELP DFIELDS -- To see a complete list of individual display fields.
HELP FORMATS -- To see detailed descriptions of the predefined formats.
ENTER DISPLAY FORMAT (IDE):
ENTER DISPLAY FORMAT (IDE):ide

L2   ANSWER 1 OF 19574  REGISTRY  COPYRIGHT 2005 ACS on STN
RN   865506-50-9  REGISTRY
ED   Entered STN:  18 Oct 2005
CN   Cytidylyltransferase, acylneuraminate (Escherichia coli strain K1
     RS218 gene neuA) (9CI)  (CA INDEX NAME)
OTHER NAMES:
CN   29: PN: WO2005090552 FIGURE: 4 claimed sequence
FS   PROTEIN SEQUENCE
MF   Unspecified
CI   MAN
SR   CA
LC   STN Files:   CA, CAPLUS

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
*** USE 'SQD' OR 'SQIDE' FORMATS TO DISPLAY SEQUENCE ***
               1 REFERENCES IN FILE CA (1907 TO DATE)
               1 REFERENCES IN FILE CAPLUS (1907 TO DATE)


=> d 1000

L2   ANSWER 1000 OF 19574  REGISTRY  COPYRIGHT 2005 ACS on STN
RN   754259-45-5  REGISTRY
ED   Entered STN:  30 Sep 2004
CN   DNA (Gossypium hirsutum clone LIB3585-038-P1-K1-G7 EST (expressed
     sequence tag)) (9CI)  (CA INDEX NAME)
OTHER NAMES:
CN   1502: PN: US20040181830 SEQID: 1502 claimed DNA
FS   NUCLEIC ACID SEQUENCE
MF   Unspecified
CI   MAN
```

SR CA
LC STN Files: CA, CAPLUS, USPATFULL

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
*** USE 'SQD' OR 'SQIDE' FORMATS TO DISPLAY SEQUENCE ***
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> d 1500

L2 ANSWER 1500 OF 19574 REGISTRY COPYRIGHT 2005 ACS on STN
RN 753049-21-7 REGISTRY
ED Entered STN: 28 Sep 2004
CN Protein (sorghum clone LIB3480-049-P1-K1-B8.pep fragment) (9CI)
(CA INDEX NAME)
OTHER NAMES:
CN 979: PN: US20040172684 SEQID: 50979 claimed protein
FS PROTEIN SEQUENCE
MF Unspecified
CI MAN
SR CA
LC STN Files: CA, CAPLUS

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
*** USE 'SQD' OR 'SQIDE' FORMATS TO DISPLAY SEQUENCE ***
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> fil caplus

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 11.41 | 12.67 |

FILE 'CAPLUS' ENTERED AT 16:58:57 ON 09 NOV 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.


FILE COVERS 1907 - 9 Nov 2005 VOL 143 ISS 20
FILE LAST UPDATED: 8 Nov 2005 (20051108/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l2

```
L3       27567 L2

=> d fhitstr

L3   ANSWER 1 OF 27567  CAPLUS  COPYRIGHT 2005 ACS on STN
IT   7681-11-0, Potassium iodide
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (synergistic topically applied personal hygiene product)
RN   7681-11-0  CAPLUS
CN   Potassium iodide (KI) (8CI, 9CI)  (CA INDEX NAME)


I—K



=> d 22000 fhitstr

L3   ANSWER 22000 OF 27567  CAPLUS  COPYRIGHT 2005 ACS on STN
IT   7681-11-0, properties
     RL: PRP (Properties)
        (electron emission from, secondary)
RN   7681-11-0  CAPLUS
CN   Potassium iodide (KI) (8CI, 9CI)  (CA INDEX NAME)


I—K



=> dis his

     (FILE 'HOME' ENTERED AT 16:53:21 ON 09 NOV 2005)

     FILE 'REGISTRY' ENTERED AT 16:56:59 ON 09 NOV 2005
L1             STRUCTURE UPLOADED
L2         19574 S K1 FUL

     FILE 'CAPLUS' ENTERED AT 16:58:57 ON 09 NOV 2005
L3         27567 S L2

=> s l3 and acetonitrile
          76750 ACETONITRILE
L4          255 L3 AND ACETONITRILE

=> d

L4   ANSWER 1 OF 255  CAPLUS  COPYRIGHT 2005 ACS on STN
AN   2005:467929  CAPLUS
DN   143:7613
TI   Simple preparation of zaltoprofen from diphenyl sulfide derivatives
IN   Nakada, Yoshitaka
PA   Ohara Pharmaceutical Co., Ltd., Japan
SO   Jpn. Kokai Tokkyo Koho, 8 pp.
     CODEN: JKXXAF
DT   Patent
LA   Japanese
```

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | JP 2005139120 | A2 | 20050602 | JP 2003-377810 | 20031107 |
| PRAI | JP 2003-377810 | | 20031107 | | |
| OS | MARPAT 143:7613 | | | | |

=> d hitstr

L4 ANSWER 1 OF 255 CAPLUS COPYRIGHT 2005 ACS on STN
IT 7681-11-0, Potassium iodide, uses
RL: CAT (Catalyst use); USES (Uses)
(preparation of zaltoprofen from alkyl acetyl(phenylthiophenyl)acetates with 4 steps)
RN 7681-11-0 CAPLUS
CN Potassium iodide (KI) (8CI, 9CI) (CA INDEX NAME)

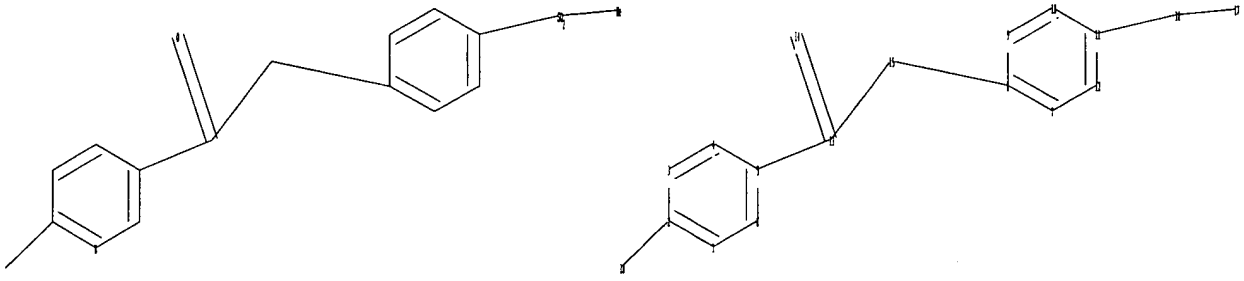
I—K

=> d 100 hitstr

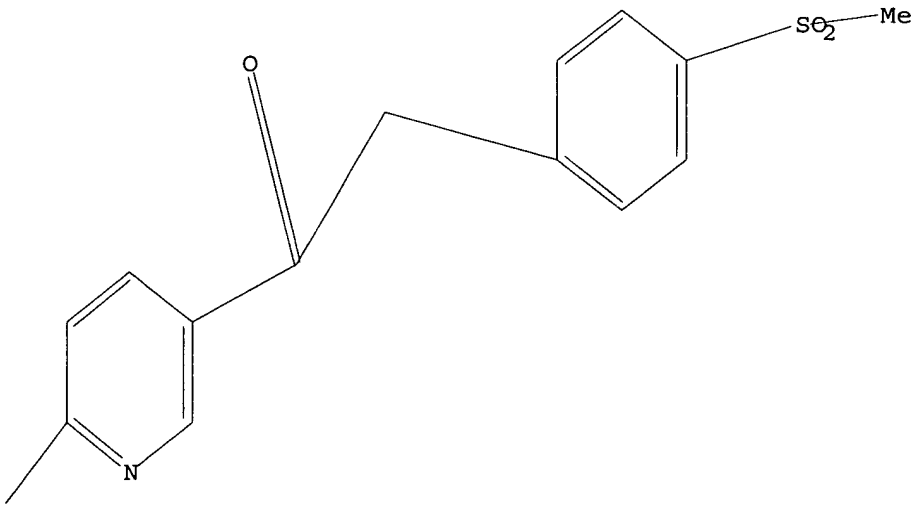
L4 ANSWER 100 OF 255 CAPLUS COPYRIGHT 2005 ACS on STN
IT 7681-11-0, Potassium iodide (KI), uses
RL: NUU (Other use, unclassified); USES (Uses)
(indirect electrolytic oxidative coupling reaction of some activated methylene compds. studied using KI-NaI as indirect electrolyte and acetone as solvent)
RN 7681-11-0 CAPLUS
CN Potassium iodide (KI) (8CI, 9CI) (CA INDEX NAME)

I—K

=>
Uploading C:\Program Files\Stnexp\Queries\rkc941.str



```
chain nodes :
13  14  15  16  17  18
ring nodes :
1  2  3  4  5  6  7  8  9  10  11  12
chain bonds :
2-18  5-13  8-15  11-16  13-14  13-15  16-17
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  7-8  7-12  8-9  9-10  10-11  11-12
exact/norm bonds :
13-14
exact bonds :
2-18  5-13  8-15  11-16  13-15  16-17
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6  7-8  7-12  8-9  9-10  10-11  11-12
isolated ring systems :
containing 1 : 7 :


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:Atom  13:CLASS  14:CLASS  15:CLASS  16:CLASS  17:CLASS  18:CLASS



L5      STRUCTURE UPLOADED

=> d
L5 HAS NO ANSWERS
L5              STR
```




```
Structure attributes must be viewed using STN Express query preparation.


=> fil reg
COST IN U.S. DOLLARS                        SINCE FILE      TOTAL
                                               ENTRY    SESSION
FULL ESTIMATED COST                            14.40      27.07

FILE 'REGISTRY' ENTERED AT 17:02:03 ON 09 NOV 2005
```

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.


Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 7 NOV 2005 HIGHEST RN 866913-62-4
DICTIONARY FILE UPDATES: 7 NOV 2005 HIGHEST RN 866913-62-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

```
**********************************************************************
*                                                                    *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,    *
* effective March 20, 2005.  A new display format, IDERL, is now     *
* available and contains the CA role and document type information. *
*                                                                    *
**********************************************************************
```

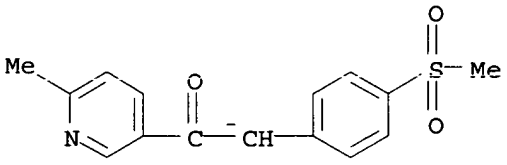
Structure search iteration limits have been increased. See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

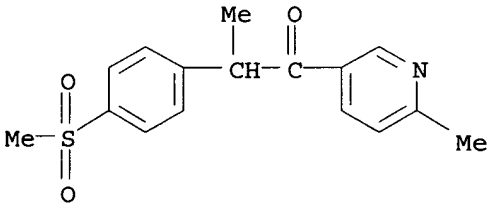
http://www.cas.org/ONLINE/UG/regprops.html

```
=> s l5
SAMPLE SEARCH INITIATED 17:02:06 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -        0 TO ITERATE

100.0% PROCESSED         0 ITERATIONS                          0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:            0 TO        0
PROJECTED ANSWERS:               0 TO        0

L6            0 SEA SSS SAM L5

=> s l5 ful
FULL SEARCH INITIATED 17:02:13 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -       20 TO ITERATE

100.0% PROCESSED        20 ITERATIONS                          4 ANSWERS
SEARCH TIME: 00.00.01

L7            4 SEA SSS FUL L5

=> d 1-4
```

L7 ANSWER 1 OF 4 REGISTRY COPYRIGHT 2005 ACS on STN
RN 788151-35-9 REGISTRY
ED Entered STN: 25 Nov 2004
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]-, ion(1-) (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H14 N O3 S
CI COM
SR CA



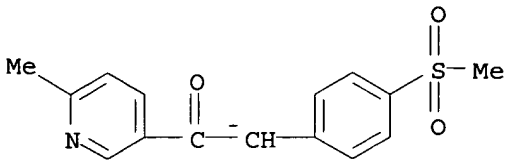
L7 ANSWER 2 OF 4 REGISTRY COPYRIGHT 2005 ACS on STN
RN 452332-13-7 REGISTRY
ED Entered STN: 18 Sep 2002
CN 1-Propanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H17 N O3 S
SR CA
LC STN Files: CA, CAPLUS



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

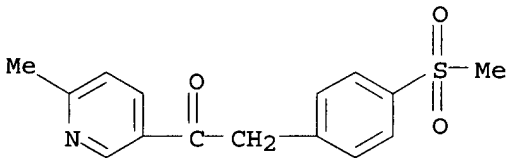
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L7 ANSWER 3 OF 4 REGISTRY COPYRIGHT 2005 ACS on STN
RN 452332-12-6 REGISTRY
ED Entered STN: 18 Sep 2002
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]-, ion(1-), potassium (9CI) (CA INDEX NAME)
MF C15 H14 N O3 S . K
SR CA
LC STN Files: CA, CAPLUS
CRN (788151-35-9)



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L7 ANSWER 4 OF 4 REGISTRY COPYRIGHT 2005 ACS on STN
RN 221615-75-4 REGISTRY
ED Entered STN: 25 Apr 1999
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone
FS 3D CONCORD
MF C15 H15 N O3 S
SR CA
LC STN Files: BIOSIS, CA, CAPLUS, CASREACT, PS, TOXCENTER, USPAT2, USPATFULL



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

16 REFERENCES IN FILE CA (1907 TO DATE)
16 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> fil caplus

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 168.69 | 195.76 |

FILE 'CAPLUS' ENTERED AT 17:02:26 ON 09 NOV 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 9 Nov 2005 VOL 143 ISS 20
FILE LAST UPDATED: 8 Nov 2005 (20051108/ED)

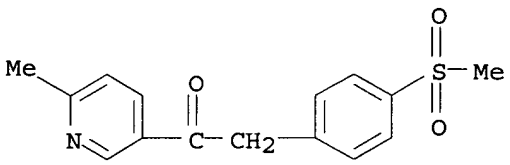
Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

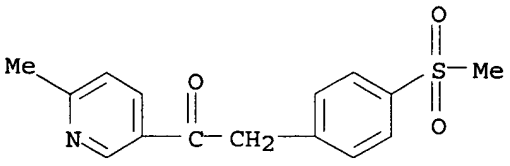
=> s l7
L8 16 L7

=> d 1-16 fhitstr

L8 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
IT 221615-75-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(review of preparation of pyridines, pyridine-1-oxides and pyridinium salts via cyclization, ring transformations, aromatization and substituent modification)
RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)

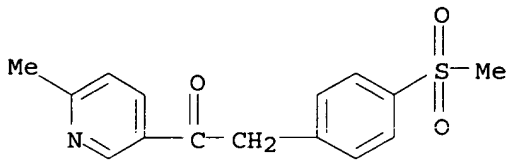



L8 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
IT 221615-75-4
RL: ANT (Analyte); PRP (Properties); ANST (Analytical study)
(development and validation of an HPLC method for the impurity and quant. anal. of etoricoxib)
RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)

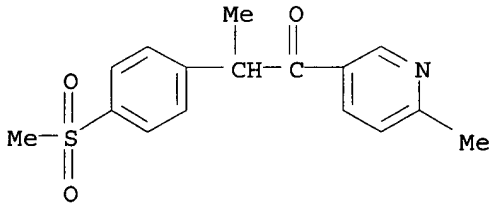



L8 ANSWER 3 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

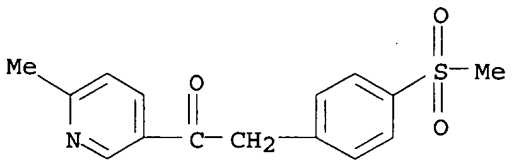
IT 221615-75-4P, 1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone
RL: IMF (Industrial manufacture); PREP (Preparation)
(production of methylpyridinyl methylsulfonylphenyl ethanone by oxidation of resp. methylthiophenyl derivative)
RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



L8 ANSWER 4 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
IT 452332-13-7
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(LC-mass spectra of)
RN 452332-13-7 CAPLUS
CN 1-Propanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)

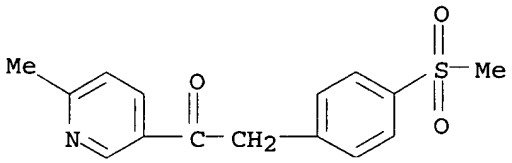


L8 ANSWER 5 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
IT 221615-75-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(treatment of cancer with prostate specific antigen (PSA) conjugate and NSAID compound)
RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)

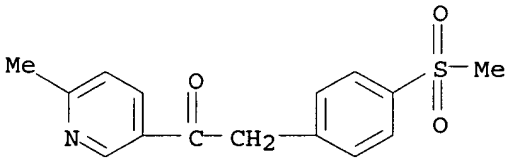


L8 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

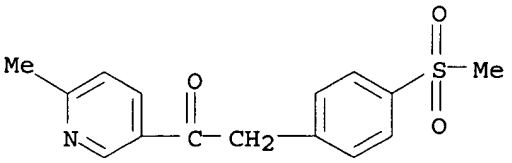
IT 221615-75-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(methanesulfonylphenylmethyl bipyridinyl in pure crystalline form and process for synthesis)
RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



L8 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
IT 221615-75-4P, 1-(6-Methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]ethanone
RL: SPN (Synthetic preparation); PREP (Preparation)
(process for the oxidation of 1-(6-methyl-3-pyridinyl)-2-[4-(methylthio)phenyl]ethanone into 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]ethanone)
RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)

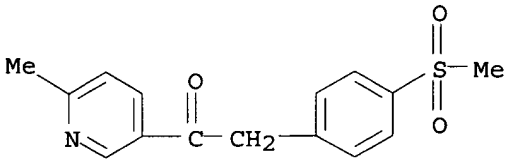


L8 ANSWER 8 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
IT 221615-75-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(process for the preparation of intermediates useful in the synthesis of diarylpyridines)
RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)

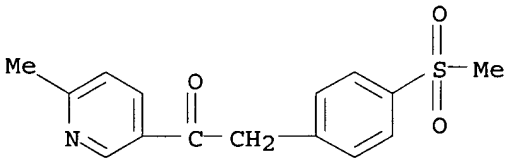


L8 ANSWER 9 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
IT 221615-75-4P

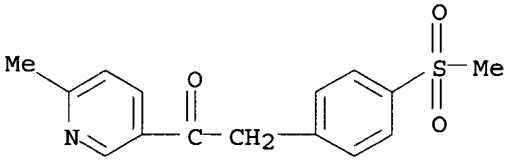
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(1,2,3-thiadiazoles as COX-2 inhibitors)
RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



L8 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
IT 221615-75-4P, 1-(6-Methylpyridin-3-yl)-2-[(4-(methylsulfonyl)phenyl]ethanone
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of 1-(6-methylpyridin-3-yl)-2-[(4-(methylsulfonyl)phenyl]ethanone starting from 4-methylthiobenzyl alc. and 6-methylnicotinate esters)
RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)

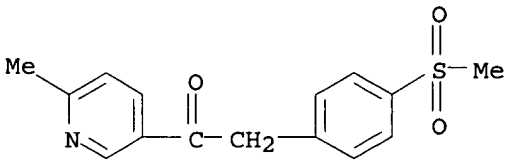


L8 ANSWER 11 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
IT 221615-75-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyridine N-oxides by cyclization of vinamidinium salts with enolates of ketones, aldehydes, and esters)
RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)

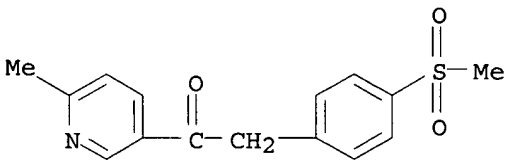


L8 ANSWER 12 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
IT 221615-75-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

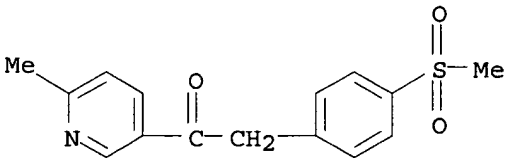
(Reactant or reagent)
(preparation of a methylsulfonylphenylbipyridine COX-2 inhibitor)
RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
(CA INDEX NAME)



L8 ANSWER 13 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
IT 221615-75-4P, 1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of 1-(6-methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone)
RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
(CA INDEX NAME)

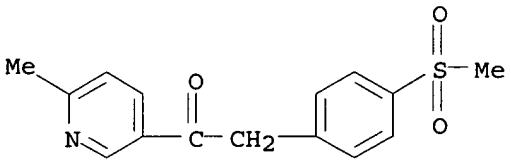


L8 ANSWER 14 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
IT 221615-75-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of trisubstituted pyridines via annulation of ketones with vinamidinium hexafluorophosphate salts)
RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI)
(CA INDEX NAME)

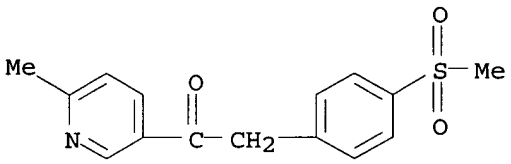


L8 ANSWER 15 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
IT 221615-75-4P, 1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of arylpyridine COX-2 inhibitors by cyclocondensation of iminium salts with ketones)
RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



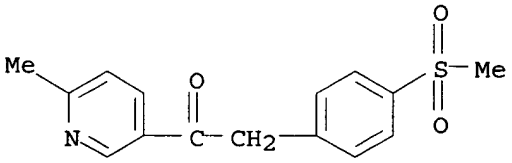
L8 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
IT 221615-75-4P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 3-phenyl-2-(3-pyridyl)pyridines and intermediates)
RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



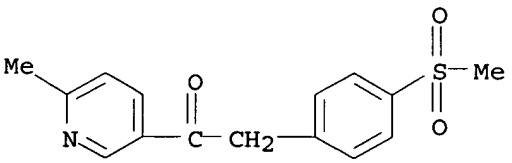
=> d 1-16 bib abs fhitstr

L8 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2005:406839 CAPLUS
Correction of: 2005:155216
DN 143:248209
Correction of: 142:197768
TI Product class 1: pyridines
AU Spitzner, D.
CS Germany
SO Science of Synthesis (2005), 15, 11-284
CODEN: SSCYJ9
PB Georg Thieme Verlag
DT Journal; General Review
LA English
AB A review of methods to prepare pyridines, pyridine-1-oxides, and pyridinium salts. Methods include cyclization, ring transformations, aromatization and substituent modification.
IT 221615-75-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(review of preparation of pyridines, pyridine-1-oxides and pyridinium salts via cyclization, ring transformations, aromatization and substituent modification)
RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



L8 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:586395 CAPLUS
DN 140:117549
TI Development and validation of an HPLC method for the impurity and quantitative analysis of etoricoxib
AU Hartman, Robert; Abrahim, Ahmed; Clausen, Andrew; Mao, Bing; Crocker, Louis S.; Ge, Zhihong
CS Analytical Research, Merck Research Laboratories, Rahway, NJ, 07065-0914, USA
SO Journal of Liquid Chromatography & Related Technologies (2003), 26(15), 2551-2566
CODEN: JLCTFC; ISSN: 1082-6076
PB Marcel Dekker, Inc.
DT Journal
LA English
AB Etoricoxib (5-chloro-6'-methyl-3[4-(methanesulfonyl)phenyl]-2,3'-bipyridine) is a highly active and selective cyclo-oxygenase II inhibitor. A single, stability-indicating HPLC method was developed and validated for both the impurity and quant. anal. of etoricoxib. Method development incorporated the optimization of stationary phase, pH, temperature, and mobile phase composition for the resolution of 13 process impurities and 3 major degradation products. Further optimization of pH and mobile phase composition was aided by the use of DryLab, a computer-based simulation program. The stability-indicating capability of the method was proven through the identification of photolytic and oxidative decomposition products. Method validation produced excellent results for linearity, precision, limit of quantitation and limit of detection, specificity, accuracy, recovery, and robustness. The identities of etoricoxib decomposition products were confirmed by UV, LC/MS, and NMR spectra.
IT 221615-75-4
RL: ANT (Analyte); PRP (Properties); ANST (Analytical study)
(development and validation of an HPLC method for the impurity and quant. anal. of etoricoxib)
RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)

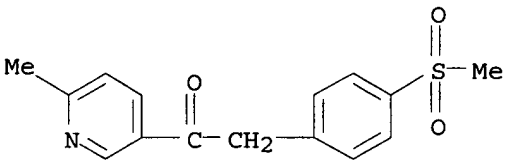


RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:491189 CAPLUS
DN 139:70705
TI Production of methylpyridinyl methylsulfonylphenyl ethanone by oxidation of the respective methylthiophenyl derivative
IN Cannata, Vincenzo; Soriato, Giorgio; Verzini, Massimo
PA Zambon Group S.P.A., Italy
SO PCT Int. Appl., 10 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

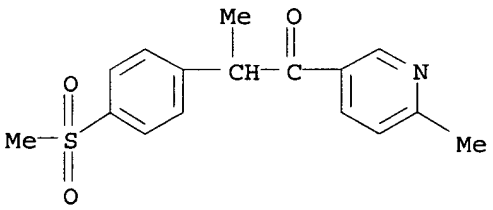
| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | WO 2003051843 | A1 | 20030626 | WO 2002-EP14115 | 20021212 |
| | W: CN, CZ, HU, IL, IN, US | | | | |
| | RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR | | | | |
| | EP 1492770 | A1 | 20050105 | EP 2002-795165 | 20021212 |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, CY, TR, BG, CZ, EE, SK | | | | |
| | US 2005165238 | A1 | 20050728 | US 2003-499321 | 20021212 |
| PRAI | IT 2001-MI2692 | A | 20011219 | | |
| | WO 2002-EP14115 | W | 20021212 | | |

OS CASREACT 139:70705
AB A process for production of 1-(6-methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone is carried out by oxidation of 1-(6-methylpyridin-3-yl)-2-[4-(methylthio)phenyl]ethanone with an oxidant in the presence of an acid, the oxidant being a mixture of peracetic acid and hydrogen peroxide, and the acid being methanesulfonic acid. The product is useful as an intermediate in production of cyclooxygenase 2 (COX 2) inhibitors. Thus, the title compound was produced in 88.6% yield by mixing 1-(6-methylpyridin-3-yl)-2-[4-(methylthio)phenyl]ethanone (30), acetic acid (45), methanesulfonic acid (13.6), adding Oxystrong (65% peracetic acid) (28.1 kg) at 35°, and reacting the mixture at 35° for 3-4 h.
IT 221615-75-4P, 1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone
RL: IMF (Industrial manufacture); PREP (Preparation)
(production of methylpyridinyl methylsulfonylphenyl ethanone by oxidation of resp. methylthiophenyl derivative)
RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)




RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 4 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2002:434902 CAPLUS
DN 137:210102
TI Development of a derivatization method, coupled with reverse phase HPLC, for monitoring the formation of an enolate intermediate
AU Abrahim, A.; Hartman, R.; Ge, Z.; Mao, B.; Marcoux, J.
CS Merck Research Laboratories, Rahway, NJ, 07065-0914, USA
SO Journal of Liquid Chromatography & Related Technologies (2002), 25(7), 1049-1062
CODEN: JLCTFC; ISSN: 1082-6076
PB Marcel Dekker, Inc.
DT Journal
LA English
AB A sensitive liquid chromatog. method was developed to monitor the formation of an enolate intermediate in a synthetic route to Etoricoxib, a drug candidate for the treatment of arthritis. The method requires the derivatization of the enolate with Me iodide to form a stable methylketosulfone derivative followed by reverse phase HPLC anal. Parameters affecting the derivatization, including the nature of derivatizing agent, reaction solvent, amount of derivatizing agent, reaction time, reaction temperature, and amount of excess base in the reaction were studied. The derivatization reaction gave selective C-alkylation. The linear range of the chromatog. method for the determination of the starting material, ketosulfone, and the derivative, methylketosulfone, was determined Finally, the accuracy of the method was established based on recovery expts.
IT 452332-13-7
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(LC-mass spectra of)
RN 452332-13-7 CAPLUS
CN 1-Propanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)




RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 5 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2002:276519 CAPLUS
DN 136:310188
TI Treatment of cancer with a prostate specific antigen (PSA) conjugate and an NSAID compound
IN Heimbrook, David C.; Yao, Siu-long
PA USA
SO U.S. Pat. Appl. Publ., 129 pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | US 2002042375 | A1 | 20020411 | US 2001-896245 | 20010629 |
| PRAI | US 2000-216217P | P | 20000705 | | |

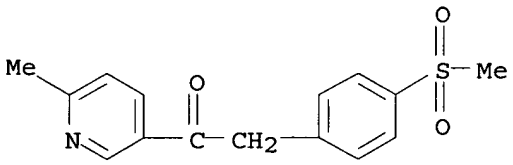
OS MARPAT 136:310188

AB The invention relates to methods of treating cancer using a combination of a compound which is a PSA conjugate and a nonsteroidal antiinflammatory agent (NSAID) and to methods of preparing such compns. The PSA conjugate comprises an oligopeptide that is selectively cleaved by PSA and a cytotoxic agent. An example of a PSA conjugate is N-Ac-(4-trans-L-Hyp)-Ala-Ser-Chg-Gln-Ser-Leu-Dox (Dox = doxorubicin, Hyp = hydroxyproline, Chg = cyclohexylglycine) and COX-2 inhibitor 3-phenyl-4-[4-(4-methylsulfonyl)phenyl]-2(5H)furanone is an example of an NSAID compound (syntheses given).

IT 221615-75-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(treatment of cancer with prostate specific antigen (PSA) conjugate and NSAID compound)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)




L8 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:886073 CAPLUS

DN 136:11103

TI 5-chloro-3-(4-methanesulfonylphenyl)-6'-methyl- [2,3']bipyridinyl in pure crystalline form and process for synthesis

IN Crocker, Louis S.; Davies, Ian W.; Osifchin, Richard G.; Kotliar, Andrew

PA Merck & Co., Inc., USA

SO PCT Int. Appl., 27 pp.
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 2

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | WO 2001092230 | A1 | 20011206 | WO 2001-US16566 | 20010522 |
| | W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| | RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| | CA 2410234 | AA | 20011206 | CA 2001-2410234 | 20010522 |
| | EP 1296951 | A1 | 20030402 | EP 2001-939267 | 20010522 |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, | | | | |

IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

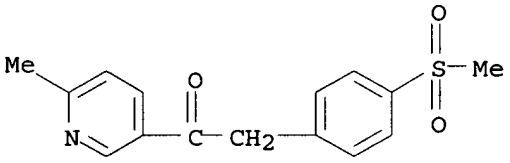
| | | | | | |
|---|---|---|---|---|---|
| | JP 2004501116 | T2 | 20040115 | JP 2002-500844 | 20010522 |
| | JP 3665053 | B2 | 20050629 | | |
| | NZ 522394 | A | 20040528 | NZ 2001-522394 | 20010522 |
| | EE 200200655 | A | 20040816 | EE 2002-655 | 20010522 |
| | BR 2001011140 | A | 20050111 | BR 2001-11140 | 20010522 |
| | BG 107237 | A | 20030530 | BG 2002-107237 | 20021031 |
| | ZA 2002009558 | A | 20031028 | ZA 2002-9558 | 20021125 |
| | JP 2005047927 | A2 | 20050224 | JP 2004-263913 | 20040910 |
| PRAI | US 2000-208017P | P | 20000526 | | |
| | JP 2002-500844 | A3 | 20010522 | | |
| | WO 2001-US16566 | W | 20010522 | | |

AB This invention encompasses the form V polymorph of the title composition which is useful in the treatment of cyclooxygenase-2 mediated diseases. The invention encompasses certain pharmaceutical compns. for treatment of cyclooxygenase-2 mediated diseases comprising the Form V polymorph of the title composition The invention also encompasses a process for synthesizing the form V polymorph of the title composition A mixture of the title composition and iso-Pr acetate was heated at 55°, then was cooled to ambient temperature and the solids were isolated by filtration. The solids were washed with iso-Pr acetate and dried in vacuo to give the form V polymorph as a colorless solid in about 87% yield.

IT 221615-75-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(methanesulfonylphenylmethyl bipyridinyl in pure crystalline form and process for synthesis)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)




RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:300685 CAPLUS

DN 134:311114

TI Process for the oxidation of 1-(6-methyl-3-pyridinyl)-2-[4-(methylthio)phenyl]ethanone into 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]ethanone

IN Cannata, Vincenzo; Rossato, Roberto

PA Zambon Group S.P.A., Italy

SO PCT Int. Appl., 9 pp.
CODEN: PIXXD2

DT Patent

LA English

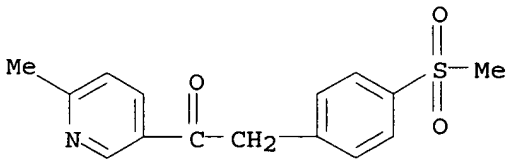
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | WO 2001029004 | A1 | 20010426 | WO 2000-EP9995 | 20001011 |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,

CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR,
HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

IT 99MI2156 A1 20010416 IT 1999-MI2156 19991015
PRAI IT 1999-MI2156 A 19991015
OS CASREACT 134:311114
AB A process for the oxidation of 1-(6-methyl-3-pyridinyl)-2-[4-(methylthio)phenyl]ethanone (I) into 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]ethanone, a pharmaceutical intermediate (no data), without the formation of N-oxide byproduct, consists of reacting I with an oxidant (e.g., a mixture of peracetic acid and hydrogen peroxide) in the presence of a catalyst (e.g., sodium tungstate) and an acid (e.g. methanesulfonic acid).
IT 221615-75-4P, 1-(6-Methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]ethanone
RL: SPN (Synthetic preparation); PREP (Preparation)
(process for the oxidation of 1-(6-methyl-3-pyridinyl)-2-[4-(methylthio)phenyl]ethanone into 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]ethanone)
RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)




RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

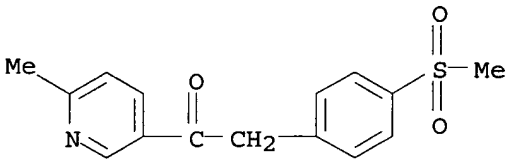
L8 ANSWER 8 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:300684 CAPLUS
DN 134:295751
TI Process for the preparation of intermediates useful in the synthesis of diarylpyridines
IN Allegrini, Pietro; Verzini, Massimo
PA Zambon Group S.P.A., Italy
SO PCT Int. Appl., 20 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| PI WO 2001029003 | A1 | 20010426 | WO 2000-EP9994 | 20001011 |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR,
HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,

YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

IT 99MI2157 A1 20010416 IT 1999-MI2157 19991015
PRAI IT 1999-MI2157 A 19991015
OS CASREACT 134:295751; MARPAT 134:295751
AB This process is used to prepare intermediates useful in the synthesis of diarylpyridines having COX-2 inhibitor activity. E.g., reaction of 6-methylnicotinic acid Me ester with (4-methylthiophenyl)acetonitrile gave 3-(6-methylpyridin-3-yl)-2-(4-methylthiophenyl)-3-oxopropionitrile hydrochloride. Acid hydrolysis and decarboxylation of the latter gave 1-(6-methylpyridin-3-yl)-2-(4-methylthiophenyl)ethanone.
IT 221615-75-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(process for the preparation of intermediates useful in the synthesis of diarylpyridines)
RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)

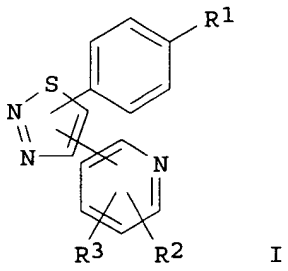



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 9 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:185752 CAPLUS
DN 134:222716
TI 1,2,3-Thiadiazoles and their use as COX-2 inhibitors
IN Lau, Cheuk K.; Li, Chun Sing; Therien, Michel; Gauthier, Jacques Y.
PA Merck Frosst Canada & Co., Can.
SO PCT Int. Appl., 45 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2001017996 | A1 | 20010315 | WO 2000-CA1040 | 20000907 |

PI WO 2001017996 A1 20010315 WO 2000-CA1040 20000907
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
PRAI US 1999-152746P P 19990908
OS MARPAT 134:222716
GI



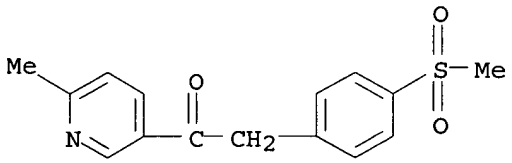
I

AB Title compds. I [R1 = SO2Me, S(O)NHMe, S(O)NHNH2, P(O)MeOH, etc.; R2, R3 = H, halo, alkoxy, alkyl, CN, etc.] were prepared Thus, 4-(6-methyl-3-pyridinyl)-5-[4-(methylsulfonyl)phenyl]-1,2,3-thiadiazole (II) was prepared in 5 steps starting from 6-methylnicotinic acid and N-methoxymethylamine hydrochloride. Oxidation of II with H2O2 gave the thiadiazole 3-oxide. Inhibition of COX-2 was determined by measuring the effects on PGE2 production in whole blood.

IT 221615-75-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(1,2,3-thiadiazoles as COX-2 inhibitors)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:78362 CAPLUS

DN 134:131435

TI Preparation of 1-(6-methylpyridin-3-yl)-2-[(4-(methylsulfonyl)phenyl]ethanone starting from 4-methylthiobenzyl alcohol and 6-methylnicotinate esters.

IN Bessard, Yves; Leresche, James Edward

PA Lonza A.-G., Switz.; Merck & Co., Inc.

SO PCT Int. Appl., 15 pp.
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| PI WO 2001007410 | A1 | 20010201 | WO 2000-EP6825 | 20000717 |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR,

HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

| | | | | | |
|---|---|---|---|---|---|
| | EP 1198455 | A1 | 20020424 | EP 2000-951393 | 20000717 |
| | EP 1198455 | B1 | 20031210 | | |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, MC, IE, SI, LT, LV, FI, RO, MK, CY, AL | | | | |
| | JP 2003505449 | T2 | 20030212 | JP 2001-512497 | 20000717 |
| | AT 256112 | E | 20031215 | AT 2000-951393 | 20000717 |
| | ES 2207536 | T3 | 20040601 | ES 2000-951393 | 20000717 |
| | US 6566527 | B1 | 20030520 | US 2002-30096 | 20020314 |
| | US 2003088107 | A1 | 20030508 | US 2002-283167 | 20021030 |
| | US 6600046 | B2 | 20030729 | | |
| PRAI | EP 1999-114667 | A | 19990727 | | |
| | US 2000-186680P | P | 20000303 | | |
| | WO 2000-EP6825 | W | 20000717 | | |
| | US 2002-30096 | A3 | 20020314 | | |

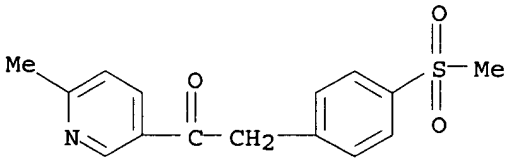
OS CASREACT 134:131435

AB 1-(6-Methylpyridin-3-yl)-2-[(4-methylsulfonyl)phenyl]ethanone was prepared by (a) treatment of 4-(methylthio)benzyl alc. with hydrochloric acid to give 4-(methylthio)benzyl chloride, (b) treatment of this with an alkali metal cyanide to give 4-(methylthio)phenylacetonitrile, (c) condensation of 4-(methylthio)phenylacetonitrile with a 6-methylnicotinate ester to give 3-[2-(4-methylthiophenyl)-2-cyanoacetyl]-6-methylpyridine, (d) hydrolysis and decarboxylation under acidic conditions to give 3-[2-(4-methylthiophenyl)acetyl]-6-methylpyridine and (e) oxidation

IT 221615-75-4P, 1-(6-Methylpyridin-3-yl)-2-[(4-(methylsulfonyl)phenyl]ethanone
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of 1-(6-methylpyridin-3-yl)-2-[(4-(methylsulfonyl)phenyl]ethanone starting from 4-methylthiobenzyl alc. and 6-methylnicotinate esters)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)




RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 11 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2000:897114 CAPLUS

DN 134:178439

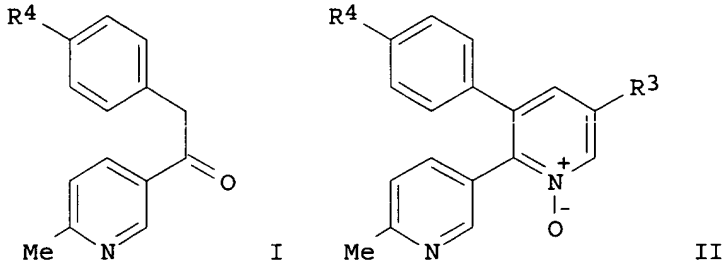
TI A general [3 + 2 + 1] annulation strategy for the preparation of pyridine N-oxides

AU Davies, Ian W.; Marcoux, Jean-Francois; Reider, Paul J.

CS Department of Process Research, Merck & Co. Inc., Rahway, NJ, 07065, USA

SO Organic Letters (2001), 3(2), 209-211

CODEN: ORLEF7; ISSN: 1523-7060
PB American Chemical Society
DT Journal
LA English
OS CASREACT 134:178439
GI

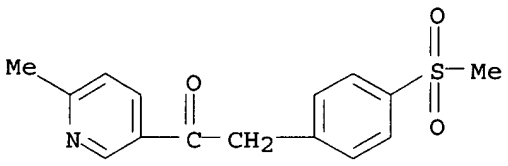



AB Stabilized ketone, aldehyde, and ester enolates, generated from I (R4 = MeSO2, MeS) for example, react with vinamidinium hexafluorophosphate salts and hydroxylamine hydrochloride to give pyridine N-oxides, e.g. II (R3 = Cl, NO2), in 45-85% yields.

IT 221615-75-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyridine N-oxides by cyclization of vinamidinium salts with enolates of ketones, aldehydes, and esters)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)




RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 12 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2000:653182 CAPLUS

DN 134:4838

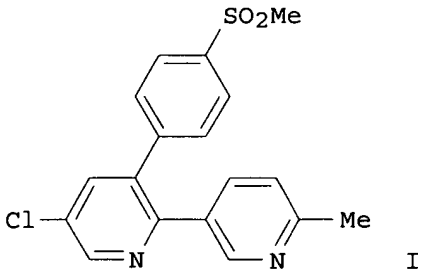
TI A Practical Synthesis of a COX-2-Specific Inhibitor

AU Davies, Ian W.; Marcoux, Jean-Francois; Corley, Edward G.; Journet, Michel; Cai, Dong-Wei; Palucki, Michael; Wu, Jimmy; Larsen, Robert D.; Rossen, Kai; Pye, Philip J.; DiMichele, Lisa; Dormer, Peter; Reider, Paul J.

CS Department of Process Research, Merck Co. Inc., Rahway, NJ, 07065, USA

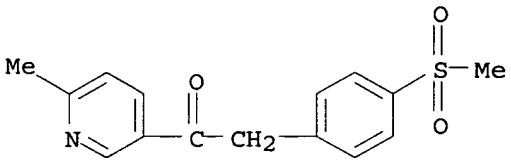
SO Journal of Organic Chemistry (2000), 65(25), 8415-8420
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal

LA English
OS CASREACT 134:4838
GI



I

AB A number of synthetic strategies to the Cox-2 specific inhibitor have been described. These studies have led to the identification of a novel pyridine construction using annulation of a ketone using a vinamidinium species and ammonia in 97% assay yield. Three approaches to the synthesis of the ketone are described that allow for its preparation in large quantities in >65% overall yield from Me 6-methylnicotinate.
IT 221615-75-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of a methylsulfonylphenylbipyridine COX-2 inhibitor)
RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



RE.CNT 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 13 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2000:493518 CAPLUS
DN 133:104966
TI Preparation of 1-(6-methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone.
IN Armbruster, Erich; Bessard, Yves; Kuo, David; Leresche, James Edward; Proplesch, Ralf; Roduit, Jean-Paul
PA Lonza A.-G., Switz.; Merck & Co., Inc.
SO PCT Int. Appl., 19 pp.
CODEN: PIXXD2
DT Patent
LA German
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | WO 2000042014 | A2 | 20000720 | WO 2000-EP240 | 20000113 |

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|---|---|---|---|---|---|
| | WO 2000042014 | A3 | 20001207 | | |
| | W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| | RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| | CA 2359958 | AA | 20000720 | CA 2000-2359958 | 20000113 |
| | CA 2485739 | AA | 20000720 | CA 2000-2485739 | 20000113 |
| | EP 1159270 | A2 | 20011205 | EP 2000-901555 | 20000113 |
| | EP 1159270 | B1 | 20031105 | | |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |
| | JP 2003518002 | T2 | 20030603 | JP 2000-593582 | 20000113 |
| | AT 253559 | E | 20031115 | AT 2000-901555 | 20000113 |
| | EP 1394149 | A1 | 20040303 | EP 2003-24787 | 20000113 |
| | EP 1394149 | B1 | 20050119 | | |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY | | | | |
| | PT 1159270 | T | 20040331 | PT 2000-901555 | 20000113 |
| | ES 2209807 | T3 | 20040701 | ES 2000-901555 | 20000113 |
| | AT 287396 | E | 20050215 | AT 2003-24787 | 20000113 |
| | PT 1394149 | T | 20050531 | PT 2003-24787 | 20000113 |
| | ES 2235138 | T3 | 20050701 | ES 2003-3024787 | 20000113 |
| | NO 2001003498 | A | 20010905 | NO 2001-3498 | 20010713 |
| | US 2005159458 | A1 | 20050721 | US 2005-29489 | 20050106 |
| PRAI | EP 1999-100590 | A | 19990114 | | |
| | US 1999-145996P | P | 19990729 | | |
| | CA 2000-2359958 | A3 | 20000113 | | |
| | EP 2000-901555 | A3 | 20000113 | | |
| | WO 2000-EP240 | W | 20000113 | | |
| | US 2003-868941 | A3 | 20031104 | | |

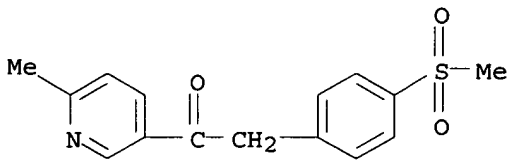
OS CASREACT 133:104966

AB 1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone (I), useful as a starting material for cyclooxygenase-2 inhibitors, was prepared Thus, N,N-diethyamino(6-methylpyridin-3-yl)acetonitrile (preparation given) and celite in PhMe were treated sequentially with aqueous NaOH, tetrabutylammonium bromide, a solution of tetrabutylammonium bromide and 4-methylsulfonylbenzyl bromide in PhMe, and tetrabutylammonium bromide followed by stirring for 6 h at 45° to give 76.4% I.

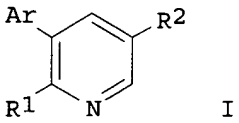
IT 221615-75-4P, 1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of 1-(6-methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



L8 ANSWER 14 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2000:443023 CAPLUS
DN 133:222553
TI Annulation of Ketones with Vinamidinium Hexafluorophosphate Salts: An Efficient Preparation of Trisubstituted Pyridines
AU Marcoux, Jean-Francois; Corley, Edward G.; Rossen, Kai; Pye, Phil; Wu, Jimmy; Robbins, Michael A.; Davies, Ian W.; Larsen, Robert D.; Reider, Paul J.
CS Department of Process Research, Merck Co. Inc., Rahway, NJ, 07065, USA
SO Organic Letters (2000), 2(15), 2339-2341
CODEN: ORLEF7; ISSN: 1523-7060
PB American Chemical Society
DT Journal
LA English
OS CASREACT 133:222553
GI

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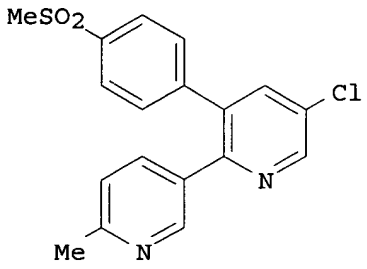
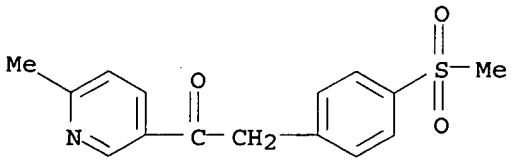



II

AB α-Aryl ketones react with vinamidinium hexafluorophosphate salts to give access to the corresponding 3-arylpyridines I (Ar = C6H4R-4, R = SO2Me, H, SMe, R1 = 6-methyl-3-pyridyl, C6H4R-4, R2 = Cl; Ar = C6H4SO2Me-4, R1 = 6-methyl-3-pyridyl, R2 = Br, I, CF3, NO2, phthalimido; Ar = C6H4F-4, R1 = Me, R2 = Cl; Ar = Ph, R1 = H, R2 = Cl). The annulation reactions proceed in good to excellent yields with vinamidinium salts containing electron-withdrawing groups at the β-position (R2). The reaction was applied to the preparation of the COX-2 specific inhibitor 5-chloro-3-(4-methylsulfonyl)phenyl-2-(2-methyl-5-pyridinyl)pyridine (II), as well as a series of analogs.
IT 221615-75-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of trisubstituted pyridines via annulation of ketones with vinamidinium hexafluorophosphate salts)
RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 15 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1999:708874 CAPLUS
DN 131:322542
TI Process for synthesizing arylpyridine COX-2 inhibitors
IN Corley, Edward G.; Davies, Ian W.; Larsen, Robert D.; Pye, Philip J.; Rossen, Kai
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 29 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | WO 9955830 | A2 | 19991104 | WO 1999-US8645 | 19990420 |
| | WO 9955830 | A3 | 19991229 | | |
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| | AU 759469 | B2 | 20030417 | AU 1999-36557 | 19990420 |
| | CZ 292515 | B6 | 20031015 | CZ 2000-3940 | 19990420 |
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| | AT 272613 | E | 20040815 | AT 1999-918706 | 19990420 |
| | PT 1071745 | T | 20041130 | PT 1999-918706 | 19990420 |
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| | WO 1999-US8645 | W | 19990420 | | |
| | US 1999-298127 | A3 | 19990423 | | |

OS CASREACT 131:322542; MARPAT 131:322542
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

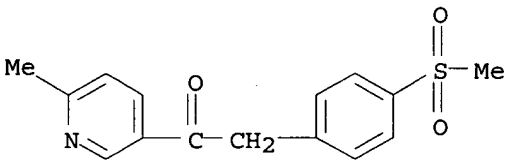
AB The invention encompasses a process and intermediates for preparing compds. I [R, R', R'' = (un)substituted alkyl, aryl, aralkyl, halo, SOmH, SOm-alkyl,

SOm-aryl, NO2, (di)(alkyl)amino, SOmNH2, SOmNH-alkyl, SOmNHCOCF3, cyano; Y = C, N; m = 0, 1, 2]. I are useful in the treatment of cyclooxygenase-2 mediated diseases (no data), i.e., as analgesics, antipyretics, and antiinflammatories. The method comprises cyclocondensation of an iminium salt II [R2-R5 = alkyl, aryl, or aralkyl; X- = suitable counterion] with an aryl ketone III in the presence of a base. The method is designed to give high yields at low temps., and with a reduced number of steps. For instance, the bipyridyl derivative IV was prepared on a 1.65-kg scale by reaction of the iminium salt V with ketone VI in THF in the presence of KOBu-tert, followed by quenching in AcOH/THF, basification with concentrated aqueous NH4OH, and refluxing. Prepns. of the salt and ketone intermediates V and VI are described, and a subset of the iminium salt intermediates II are claimed per se.

IT 221615-75-4P, 1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of arylpyridine COX-2 inhibitors by cyclocondensation of iminium salts with ketones)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)




L8 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1999:222917 CAPLUS

DN 130:252250

TI Preparation of 3-phenyl-2-(3-pyridyl)pyridines and intermediates.

IN Davies, Ian W.; Gerena, Linda; Journet, Michel; Larsen, Robert D.; Pye, Philip J.; Rossen, Kai

PA Merck & Co., Inc., USA

SO PCT Int. Appl., 42 pp.
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
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| | CN 1134414 | B | 20040114 | CN 1998-811147 | 19980922 |
| | SK 283811 | B6 | 20040203 | SK 2000-422 | 19980922 |
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| | HK 1029343 | A1 | 20030502 | HK 2001-100155 | 20010106 |
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| | GB 1998-6419 | A | 19980325 | | |
| | WO 1998-US19788 | W | 19980922 | | |
| | US 2000-509230 | A3 | 20000323 | | |

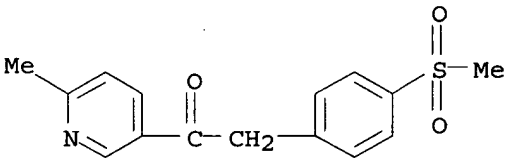
OS CASREACT 130:252250; MARPAT 130:252250

AB P-(ArCOCH2)C6H4SO2R1 (R1 = Me, NH2, NHCOCF3, NHMe; Ar = mono-, di-, or trisubstituted Ph, pyridyl, N-oxide thereof), were prepared by reaction of p-MeSC6H4CH2MgX (X = Cl, Br, F, iodo) with ArCONMe2 (Ar as above) to give p-(ArCOCH2)C6H4SMe followed by oxidation of the latter. Thus, the Grignard reagent from p-MeSC6H4CH2Cl in PhMe/THF was added to a -20° solution of 6-methylnicotinic acid N-methyl-N-methoxyamide (preparation given) in PhMe over 30 min. followed by 1 h aging to give 76% 2-methyl-5-(4-methylthiophenylacetyl)pyridine. The latter in MeOH/H2SO4 at 55° was treated with aqueous Na tungstate and then with H2O2 over 1 h to give 82.5% 2-methyl-5-(4-methylsulfonylphenylacetyl)pyridine. The latter reacted with 3-amino-2-chloroacrolein (preparation given) to give 65% 5-chloro-2-(2-methylpyrid-5-yl)-3-(4-methylsulfonylphenyl)pyridine.

IT 221615-75-4P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 3-phenyl-2-(3-pyridyl)pyridines and intermediates)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)

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COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

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L8   ANSWER 16 OF 16  CAPLUS  COPYRIGHT 2005 ACS on STN
AN   1999:222917  CAPLUS
DN   130:252250
TI   Preparation of 3-phenyl-2-(3-pyridyl)pyridines and intermediates.
IN   Davies, Ian W.; Gerena, Linda; Journet, Michel; Larsen, Robert D.; Pye,
     Philip J.; Rossen, Kai
PA   Merck & Co., Inc., USA
SO   PCT Int. Appl., 42 pp.
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     CODEN: PIXXD2
DT   Patent
LA   English
FAN.CNT 1
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     EP 1023266             A2    20000802    EP 1998-948426           19980922
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     JP 3325263             B2    20020917
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     ES 2189251             T3    20030701    ES 1998-948426           19980922
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OS   CASREACT 130:252250; MARPAT 130:252250


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AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Nov  4, 2005 (20051104/UP).

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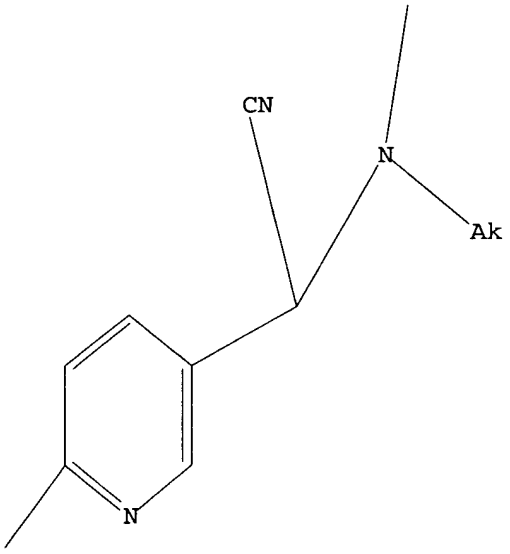


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CN   3-Pyridineacetonitrile, α-(diethylamino)-6-methyl- (9CI)  (CA INDEX
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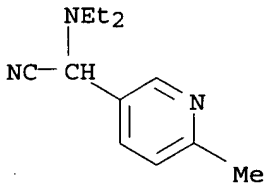


**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

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FILE COVERS 1907 - 10 Nov 2005 VOL 143 ISS 20
FILE LAST UPDATED: 9 Nov 2005 (20051109/ED)

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They are available for your review at:

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L3 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2000:493518 CAPLUS
DN 133:104966
TI Preparation of 1-(6-methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone.

IN Armbruster, Erich; Bessard, Yves; Kuo, David; Leresche, James Edward; Proplesch, Ralf; Roduit, Jean-Paul
PA Lonza A.-G., Switz.; Merck & Co., Inc.
SO PCT Int. Appl., 19 pp.
CODEN: PIXXD2
DT Patent
LA German
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | | DATE |
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| PI | WO 2000042014 | A2 | 20000720 | WO 2000-EP240 | | 20000113 |
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STRUCTURE FILE UPDATES: 8 NOV 2005 HIGHEST RN 866995-49-5
DICTIONARY FILE UPDATES: 8 NOV 2005 HIGHEST RN 866995-49-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

**********
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*
**********

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

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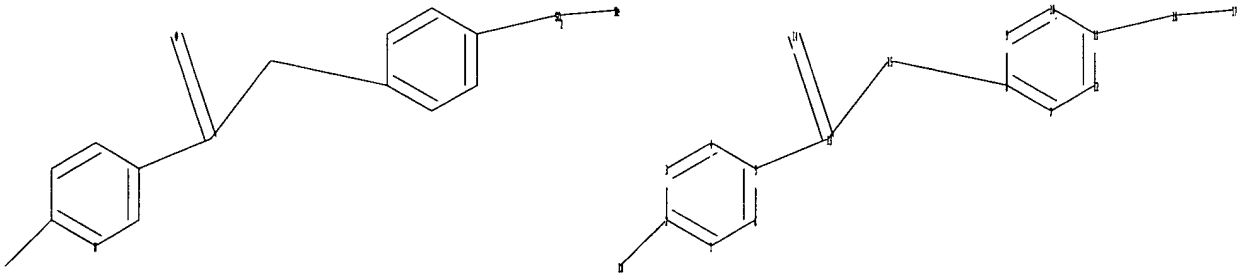
Uploading C:\Program Files\Stnexp\Queries\rkc941.str



chain nodes :
13 14 15 16 17 18
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
2-18 5-13 8-15 11-16 13-14 13-15 16-17
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
13-14
exact bonds :
2-18 5-13 8-15 11-16 13-15 16-17

normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
isolated ring systems :
containing 1 : 7 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS

L4 STRUCTURE UPLOADED

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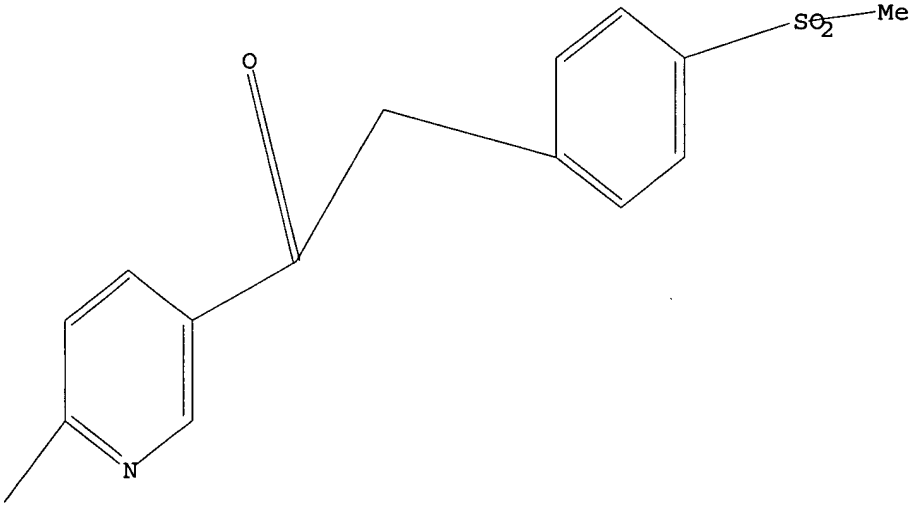
L4 HAS NO ANSWERS
L4 STR




Structure attributes must be viewed using STN Express query preparation.

=> s l4 ful
FULL SEARCH INITIATED 15:43:42 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 20 TO ITERATE

100.0% PROCESSED 20 ITERATIONS 4 ANSWERS
SEARCH TIME: 00.00.01

L5 4 SEA SSS FUL L4

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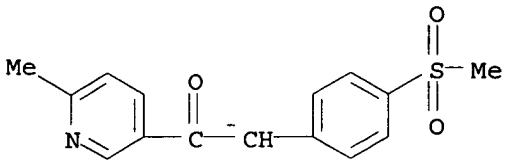
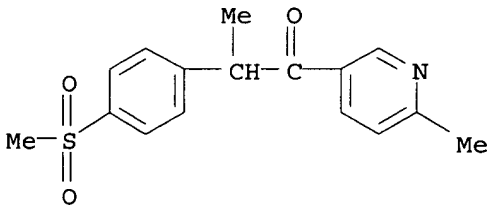
L5 ANSWER 1 OF 4 REGISTRY COPYRIGHT 2005 ACS on STN
RN 788151-35-9 REGISTRY
ED Entered STN: 25 Nov 2004
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]-, ion(1-)
(9CI) (CA INDEX NAME)
FS 3D CONCORD

MF C15 H14 N O3 S
CI COM
SR CA



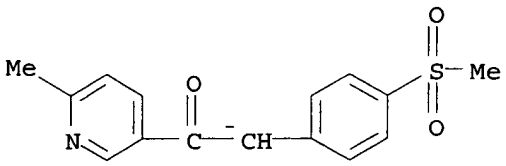
L5 ANSWER 2 OF 4 REGISTRY COPYRIGHT 2005 ACS on STN
RN 452332-13-7 REGISTRY
ED Entered STN: 18 Sep 2002
CN 1-Propanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H17 N O3 S
SR CA
LC STN Files: CA, CAPLUS



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

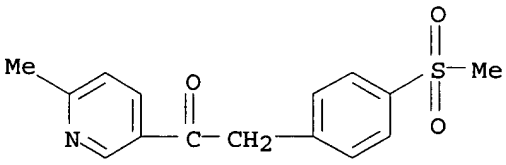
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 3 OF 4 REGISTRY COPYRIGHT 2005 ACS on STN
RN 452332-12-6 REGISTRY
ED Entered STN: 18 Sep 2002
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]-, ion(1-), potassium (9CI) (CA INDEX NAME)
MF C15 H14 N O3 S . K
SR CA
LC STN Files: CA, CAPLUS
CRN (788151-35-9)



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 4 OF 4 REGISTRY COPYRIGHT 2005 ACS on STN
RN 221615-75-4 REGISTRY
ED Entered STN: 25 Apr 1999
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone
FS 3D CONCORD
MF C15 H15 N O3 S
SR CA
LC STN Files: BIOSIS, CA, CAPLUS, CASREACT, PS, TOXCENTER, USPAT2, USPATFULL



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

16 REFERENCES IN FILE CA (1907 TO DATE)
16 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> fil caplus

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|---|---|---|
| FULL ESTIMATED COST | 168.69 | 338.36 |

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| CA SUBSCRIBER PRICE | 0.00 | -0.73 |

FILE 'CAPLUS' ENTERED AT 15:43:52 ON 10 NOV 2005
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FILE COVERS 1907 - 10 Nov 2005 VOL 143 ISS 20
FILE LAST UPDATED: 9 Nov 2005 (20051109/ED)

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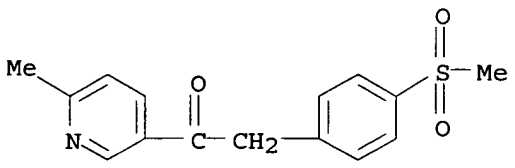
http://www.cas.org/infopolicy.html

=> s l5
L6 16 L5

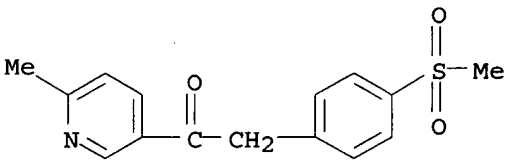
=> d 1-16 fbib abs fhitstr

L6 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2005:406839 CAPLUS
Correction of: 2005:155216
DN 143:248209
Correction of: 142:197768
TI Product class 1: pyridines
AU Spitzner, D.
CS Germany
SO Science of Synthesis (2005), 15, 11-284
CODEN: SSCYJ9
PB Georg Thieme Verlag
DT Journal; General Review
LA English
AB A review of methods to prepare pyridines, pyridine-1-oxides, and pyridinium salts. Methods include cyclization, ring transformations, aromatization and substituent modification.
IT 221615-75-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(review of preparation of pyridines, pyridine-1-oxides and pyridinium salts via cyclization, ring transformations, aromatization and substituent modification)
RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)




L6 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2003:586395 CAPLUS
DN 140:117549
TI Development and validation of an HPLC method for the impurity and quantitative analysis of etoricoxib
AU Hartman, Robert; Abrahim, Ahmed; Clausen, Andrew; Mao, Bing; Crocker, Louis S.; Ge, Zhihong
CS Analytical Research, Merck Research Laboratories, Rahway, NJ, 07065-0914, USA
SO Journal of Liquid Chromatography & Related Technologies (2003), 26(15), 2551-2566
CODEN: JLCTFC; ISSN: 1082-6076
PB Marcel Dekker, Inc.
DT Journal
LA English
AB Etoricoxib (5-chloro-6'-methyl-3[4-(methanesulfonyl)phenyl]-2,3'-bipyridine) is a highly active and selective cyclo-oxygenase II inhibitor. A single, stability-indicating HPLC method was developed and validated for both the impurity and quant. anal. of etoricoxib. Method development incorporated the optimization of stationary phase, pH, temperature, and mobile phase composition for the resolution of 13 process impurities and 3 major degradation products. Further optimization of pH and mobile phase composition was aided by the use of DryLab, a computer-based simulation program. The stability-indicating capability of the method was proven through the identification of photolytic and oxidative decomposition products. Method validation produced excellent results for linearity, precision, limit of quantitation and limit of detection, specificity, accuracy, recovery, and robustness. The identities of etoricoxib decomposition products were confirmed by UV, LC/MS, and NMR spectra.
IT 221615-75-4
RL: ANT (Analyte); PRP (Properties); ANST (Analytical study)
(development and validation of an HPLC method for the impurity and quant. anal. of etoricoxib)
RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)




RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:491189 CAPLUS
DN 139:70705
TI Production of methylpyridinyl methylsulfonylphenyl ethanone by oxidation of the respective methylthiophenyl derivative
IN Cannata, Vincenzo; Soriato, Giorgio; Verzini, Massimo
PA Zambon Group S.P.A., Italy
SO PCT Int. Appl., 10 pp.
CODEN: PIXXD2
DT Patent
LA English

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | | DATE |
|---|---|---|---|---|---|---|
| PI | WO 2003051843 | A1 | 20030626 | WO 2002-EP14115 | | 20021212 |
| | W: CN, CZ, HU, IL, IN, US | | | | | |
| | RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR | | | | | |
| | | | | IT 2001-MI2692 | A | 20011219 |
| | EP 1492770 | A1 | 20050105 | EP 2002-795165 | | 20021212 |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, CY, TR, BG, CZ, EE, SK | | | | | |
| | | | | IT 2001-MI2692 | A | 20011219 |
| | | | | WO 2002-EP14115 | W | 20021212 |
| | US 2005165238 | A1 | 20050728 | US 2003-499321 | | 20021212 |
| | | | | IT 2001-MI2692 | A | 20011219 |
| | | | | WO 2002-EP14115 | W | 20021212 |

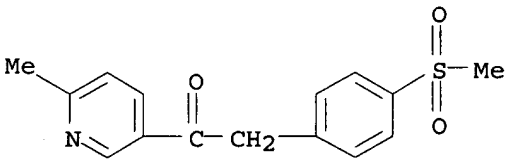
OS CASREACT 139:70705

AB A process for production of 1-(6-methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone is carried out by oxidation of 1-(6-methylpyridin-3-yl)-2-[4-(methylthio)phenyl]ethanone with an oxidant in the presence of an acid, the oxidant being a mixture of peracetic acid and hydrogen peroxide, and the acid being methanesulfonic acid. The product is useful as an intermediate in production of cyclooxygenase 2 (COX 2) inhibitors. Thus, the title compound was produced in 88.6% yield by mixing 1-(6-methylpyridin-3-yl)-2-[4-(methylthio)phenyl]ethanone (30), acetic acid (45), methanesulfonic acid (13.6), adding Oxystrong (65% peracetic acid) (28.1 kg) at 35°, and reacting the mixture at 35° for 3-4 h.

IT 221615-75-4P, 1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone
RL: IMF (Industrial manufacture); PREP (Preparation)
(production of methylpyridinyl methylsulfonylphenyl ethanone by oxidation of resp. methylthiophenyl derivative)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)




RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2002:434902 CAPLUS

DN 137:210102

TI Development of a derivatization method, coupled with reverse phase HPLC, for monitoring the formation of an enolate intermediate

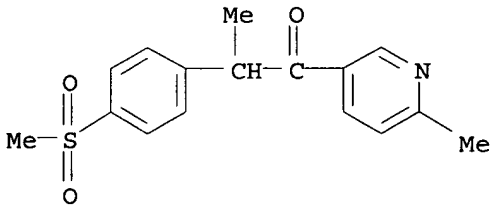
AU Abrahim, A.; Hartman, R.; Ge, Z.; Mao, B.; Marcoux, J.

CS Merck Research Laboratories, Rahway, NJ, 07065-0914, USA

SO Journal of Liquid Chromatography & Related Technologies (2002), 25(7), 1049-1062
CODEN: JLCTFC; ISSN: 1082-6076

PB Marcel Dekker, Inc.

DT Journal
LA English
AB A sensitive liquid chromatog. method was developed to monitor the formation of an enolate intermediate in a synthetic route to Etoricoxib, a drug candidate for the treatment of arthritis. The method requires the derivatization of the enolate with Me iodide to form a stable methylketosulfone derivative followed by reverse phase HPLC anal. Parameters affecting the derivatization, including the nature of derivatizing agent, reaction solvent, amount of derivatizing agent, reaction time, reaction temperature, and amount of excess base in the reaction were studied. The derivatization reaction gave selective C-alkylation. The linear range of the chromatog. method for the determination of the starting material, ketosulfone, and the derivative, methylketosulfone, was determined Finally, the accuracy of the method was established based on recovery expts.
IT 452332-13-7
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(LC-mass spectra of)
RN 452332-13-7 CAPLUS
CN 1-Propanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2002:276519 CAPLUS
DN 136:310188
TI Treatment of cancer with a prostate specific antigen (PSA) conjugate and an NSAID compound
IN Heimbrook, David C.; Yao, Siu-long
PA USA
SO U.S. Pat. Appl. Publ., 129 pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | | DATE |
|---|---|---|---|---|---|
| PI US 2002042375 | A1 | 20020411 | US 2001-896245 | | 20010629 |
| | | | US 2000-216217P | P | 20000705 |

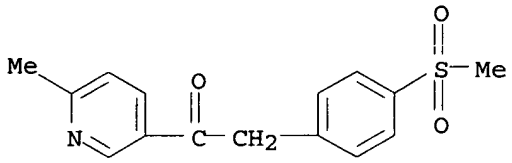
OS MARPAT 136:310188
AB The invention relates to methods of treating cancer using a combination of a compound which is a PSA conjugate and a nonsteroidal antiinflammatory agent (NSAID) and to methods of preparing such compns. The PSA conjugate comprises an oligopeptide that is selectively cleaved by PSA and a cytotoxic agent. An example of a PSA conjugate is N-Ac-(4-trans-L-Hyp)-Ala-Ser-Chg-Gln-Ser-Leu-Dox (Dox = doxorubicin, Hyp = hydroxyproline, Chg

= cyclohexylglycine) and COX-2 inhibitor 3-phenyl-4-[4-(4-methylsulfonyl)phenyl]-2(5H)furanone is an example of an NSAID compound (syntheses given).

IT 221615-75-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(treatment of cancer with prostate specific antigen (PSA) conjugate and NSAID compound)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)




L6 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:886073 CAPLUS

DN 136:11103

TI 5-chloro-3-(4-methanesulfonylphenyl)-6'-methyl- [2,3']bipyridinyl in pure crystalline form and process for synthesis

IN Crocker, Louis S.; Davies, Ian W.; Osifchin, Richard G.; Kotliar, Andrew

PA Merck & Co., Inc., USA

SO PCT Int. Appl., 27 pp.
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 2

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
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| PI | WO 2001092230 | A1 | 20011206 | WO 2001-US16566 | 20010522 |
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| | RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| | | | | US 2000-208017P | P 20000526 |
| | CA 2410234 | AA | 20011206 | CA 2001-2410234 | 20010522 |
| | | | | US 2000-208017P | P 20000526 |
| | | | | WO 2001-US16566 | W 20010522 |
| | EP 1296951 | A1 | 20030402 | EP 2001-939267 | 20010522 |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | | | |
| | | | | US 2000-208017P | P 20000526 |
| | | | | WO 2001-US16566 | W 20010522 |
| | JP 2004501116 | T2 | 20040115 | JP 2002-500844 | 20010522 |
| | JP 3665053 | B2 | 20050629 | | |
| | | | | US 2000-208017P | P 20000526 |
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| | NZ 522394 | A | 20040528 | NZ 2001-522394 | 20010522 |

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| | | | | US 2000-208017P | P | 20000526 |
| | | | | WO 2001-US16566 | W | 20010522 |
| | EE 200200655 | A | 20040816 | EE 2002-655 | | 20010522 |
| | | | | US 2000-208017P | P | 20000526 |
| | | | | WO 2001-US16566 | W | 20010522 |
| | BR 2001011140 | A | 20050111 | BR 2001-11140 | | 20010522 |
| | | | | US 2000-208017P | P | 20000526 |
| | | | | WO 2001-US16566 | W | 20010522 |
| | BG 107237 | A | 20030530 | BG 2002-107237 | | 20021031 |
| | | | | US 2000-208017P | P | 20000526 |
| | | | | WO 2001-US16566 | W | 20010522 |
| | ZA 2002009558 | A | 20031028 | ZA 2002-9558 | | 20021125 |
| | | | | US 2000-208017P | P | 20000526 |
| | JP 2005047927 | A2 | 20050224 | JP 2004-263913 | | 20040910 |
| | | | | US 2000-208017P | P | 20000526 |
| | | | | JP 2002-500844 | A3 | 20010522 |

PATENT FAMILY INFORMATION:

FAN 2002:778724

| | PATENT NO. | KIND | DATE | APPLICATION NO. | | DATE |
|---|---|---|---|---|---|---|
| PI | US 2002147221 | A1 | 20021010 | US 2001-957966 | | 20010921 |
| | US 6800647 | B2 | 20041005 | | | |
| | | | | US 2000-208017P | P | 20000526 |
| | | | | US 2001-865771 | A2 | 20010525 |
| | US 2002016343 | A1 | 20020207 | US 2001-865771 | | 20010525 |
| | US 6521642 | B2 | 20030218 | | | |
| | | | | US 2000-208017P | P | 20000526 |
| | CA 2447878 | AA | 20021205 | CA 2001-2447878 | | 20010921 |
| | | | | US 2001-865771 | A | 20010525 |
| | | | | WO 2001-US29551 | W | 20010921 |
| | WO 2002096877 | A1 | 20021205 | WO 2001-US29551 | | 20010921 |
| | W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | | |
| | RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | | |
| | | | | US 2001-865771 | A | 20010525 |
| | EP 1395562 | A1 | 20040310 | EP 2001-973314 | | 20010921 |
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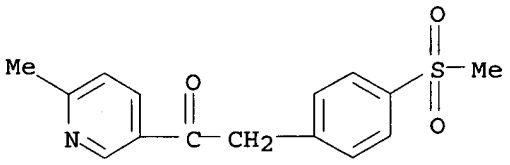
| | | | | US 2001-865771 | A | 20010525 |
| | | | | WO 2001-US29551 | W | 20010921 |
| | JP 2004530706 | T2 | 20041007 | JP 2003-500057 | | 20010921 |
| | | | | US 2001-865771 | A | 20010525 |
| | | | | WO 2001-US29551 | W | 20010921 |
| | US 2003153600 | A1 | 20030814 | US 2003-342380 | | 20030114 |
| | US 6673935 | B2 | 20040106 | | | |
| | | | | US 2001-865771 | A3 | 20010525 |
| | JP 2005047927 | A2 | 20050224 | JP 2004-263913 | | 20040910 |
| | | | | US 2000-208017P | P | 20000526 |
| | | | | JP 2002-500844 | A3 | 20010522 |

AB This invention encompasses the form V polymorph of the title composition which is useful in the treatment of cyclooxygenase-2 mediated diseases. The invention encompasses certain pharmaceutical compns. for treatment of cyclooxygenase-2 mediated diseases comprising the Form V polymorph of the title composition The invention also encompasses a process for synthesizing

the form V polymorph of the title composition A mixture of the title composition and
iso-Pr acetate was heated at 55°, then was cooled to ambient temperature and the solids were isolated by filtration. The solids were washed with iso-Pr acetate and dried in vacuo to give the form V polymorph as a colorless solid in about 87% yield.

IT 221615-75-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(methanesulfonylphenylmethyl bipyridinyl in pure crystalline form and process for synthesis)

RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)




RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:300685 CAPLUS
DN 134:311114
TI Process for the oxidation of 1-(6-methyl-3-pyridinyl)-2-[4-(methylthio)phenyl]ethanone into 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]ethanone
IN Cannata, Vincenzo; Rossato, Roberto
PA Zambon Group S.P.A., Italy
SO PCT Int. Appl., 9 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| PI WO 2001029004 | A1 | 20010426 | WO 2000-EP9995 | 20001011 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| | | | IT 1999-MI2156 | A 19991015 |
| IT 99MI2156 | A1 | 20010416 | IT 1999-MI2156 | 19991015 |

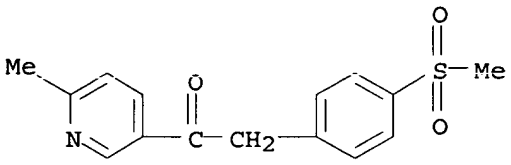
OS CASREACT 134:311114
AB A process for the oxidation of 1-(6-methyl-3-pyridinyl)-2-[4-(methylthio)phenyl]ethanone (I) into 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]ethanone, a pharmaceutical intermediate (no data), without the formation of N-oxide byproduct, consists of reacting I with an oxidant (e.g., a mixture of peracetic acid and hydrogen peroxide) in the presence of a catalyst (e.g., sodium tungstate) and an acid (e.g.

methanesulfonic acid).

IT 221615-75-4P, 1-(6-Methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]ethanone
RL: SPN (Synthetic preparation); PREP (Preparation)
(process for the oxidation of 1-(6-methyl-3-pyridinyl)-2-[4-(methylthio)phenyl]ethanone into 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]ethanone)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)




RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 8 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:300684 CAPLUS

DN 134:295751

TI Process for the preparation of intermediates useful in the synthesis of diarylpyridines

IN Allegrini, Pietro; Verzini, Massimo

PA Zambon Group S.P.A., Italy

SO PCT Int. Appl., 20 pp.
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

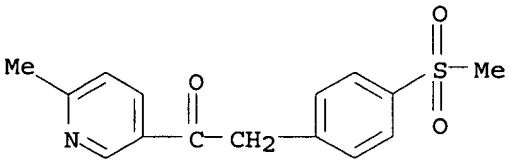
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| PI WO 2001029003 | A1 | 20010426 | WO 2000-EP9994 | 20001011 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| | | | IT 1999-MI2157 | A 19991015 |
| IT 99MI2157 | A1 | 20010416 | IT 1999-MI2157 | 19991015 |

OS CASREACT 134:295751; MARPAT 134:295751

AB This process is used to prepare intermediates useful in the synthesis of diarylpyridines having COX-2 inhibitor activity. E.g., reaction of 6-methylnicotinic acid Me ester with (4-methylthiophenyl)acetonitrile gave 3-(6-methylpyridin-3-yl)-2-(4-methylthiophenyl)-3-oxopropionitrile hydrochloride. Acid hydrolysis and decarboxylation of the latter gave 1-(6-methylpyridin-3-yl)-2-(4-methylthiophenyl)ethanone.

IT 221615-75-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(process for the preparation of intermediates useful in the synthesis of diarylpyridines)

RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

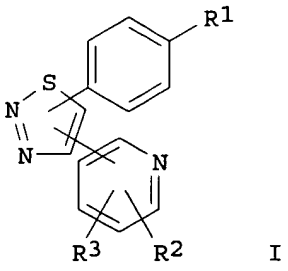
L6 ANSWER 9 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:185752 CAPLUS
DN 134:222716
TI 1,2,3-Thiadiazoles and their use as COX-2 inhibitors
IN Lau, Cheuk K.; Li, Chun Sing; Therien, Michel; Gauthier, Jacques Y.
PA Merck Frosst Canada & Co., Can.
SO PCT Int. Appl., 45 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| PI WO 2001017996 | A1 | 20010315 | WO 2000-CA1040 | 20000907 |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

US 1999-152746P P 19990908

OS MARPAT 134:222716
GI



I

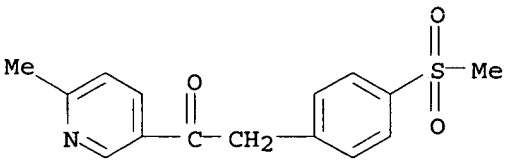
AB Title compds. I [R1 = SO2Me, S(O)NHMe, S(O)NHNH2, P(O)MeOH, etc.; R2, R3 = H, halo, alkoxy, alkyl, CN, etc.] were prepared Thus, 4-(6-methyl-3-pyridinyl)-5-[4-(methylsulfonyl)phenyl]-1,2,3-thiadiazole (II) was prepared

in 5 steps starting from 6-methylnicotinic acid and N-methoxymethylamine hydrochloride. Oxidation of II with H2O2 gave the thiadiazole 3-oxide. Inhibition of COX-2 was determined by measuring the effects on PGE2 production in whole blood.

IT 221615-75-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(1,2,3-thiadiazoles as COX-2 inhibitors)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:78362 CAPLUS

DN 134:131435

TI Preparation of 1-(6-methylpyridin-3-yl)-2-[(4-(methylsulfonyl)phenyl]ethanone starting from 4-methylthiobenzyl alcohol and 6-methylnicotinate esters.

IN Bessard, Yves; Leresche, James Edward

PA Lonza A.-G., Switz.; Merck & Co., Inc.

SO PCT Int. Appl., 15 pp.
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| PI WO 2001007410 | A1 | 20010201 | WO 2000-EP6825 | 20000717 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| | | | EP 1999-114667 | A 19990727 |
| | | | US 2000-186680P | P 20000303 |
| EP 1198455 | A1 | 20020424 | EP 2000-951393 | 20000717 |
| EP 1198455 | B1 | 20031210 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, MC, IE, SI, LT, LV, FI, RO, MK, CY, AL | | | | |
| | | | EP 1999-114667 | A 19990727 |
| | | | US 2000-186680P | P 20000303 |
| | | | WO 2000-EP6825 | W 20000717 |
| JP 2003505449 | T2 | 20030212 | JP 2001-512497 | 20000717 |

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|---|---|---|---|---|---|---|
| | | | | EP 1999-114667 | A | 19990727 |
| | | | | US 2000-186680P | P | 20000303 |
| | | | | WO 2000-EP6825 | W | 20000717 |
| | AT 256112 | E | 20031215 | AT 2000-951393 | | 20000717 |
| | | | | EP 1999-114667 | A | 19990727 |
| | | | | US 2000-186680P | P | 20000303 |
| | | | | WO 2000-EP6825 | W | 20000717 |
| | ES 2207536 | T3 | 20040601 | ES 2000-951393 | | 20000717 |
| | | | | EP 1999-114667 | A | 19990727 |
| | | | | US 2000-186680P | P | 20000303 |
| | US 6566527 | B1 | 20030520 | US 2002-30096 | | 20020314 |
| | | | | EP 1999-114667 | A | 19990727 |
| | | | | US 2000-186680P | P | 20000303 |
| | | | | WO 2000-EP6825 | W | 20000717 |
| | US 2003088107 | A1 | 20030508 | US 2002-283167 | | 20021030 |
| | US 6600046 | B2 | 20030729 | | | |
| | | | | EP 1999-114667 | A | 19990727 |
| | | | | US 2000-186680P | P | 20000303 |
| | | | | WO 2000-EP6825 | W | 20000717 |
| | | | | US 2002-30096 | A3 | 20020314 |

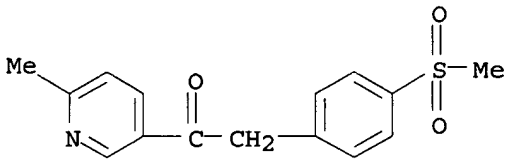
OS CASREACT 134:131435

AB 1-(6-Methylpyridin-3-yl)-2-[(4-methylsulfonyl)phenyl]ethanone was prepared by (a) treatment of 4-(methylthio)benzyl alc. with hydrochloric acid to give 4-(methylthio)benzyl chloride, (b) treatment of this with an alkali metal cyanide to give 4-(methylthio)phenylacetonitrile, (c) condensation of 4-(methylthio)phenylacetonitrile with a 6-methylnicotinate ester to give 3-[2-(4-methylthiophenyl)-2-cyanoacetyl]-6-methylpyridine, (d) hydrolysis and decarboxylation under acidic conditions to give 3-[2-(4-methylthiophenyl)acetyl]-6-methylpyridine and (e) oxidation

IT 221615-75-4P, 1-(6-Methylpyridin-3-yl)-2-[(4-(methylsulfonyl)phenyl]ethanone
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of 1-(6-methylpyridin-3-yl)-2-[(4-(methylsulfonyl)phenyl]ethanone starting from 4-methylthiobenzyl alc. and 6-methylnicotinate esters)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)




RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 11 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2000:897114 CAPLUS

DN 134:178439

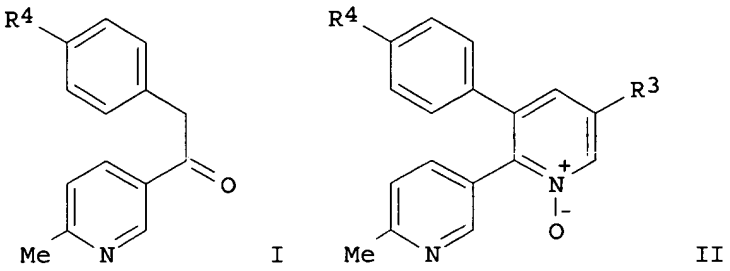
TI A general [3 + 2 + 1] annulation strategy for the preparation of pyridine N-oxides

AU Davies, Ian W.; Marcoux, Jean-Francois; Reider, Paul J.

CS Department of Process Research, Merck & Co. Inc., Rahway, NJ, 07065, USA

SO Organic Letters (2001), 3(2), 209-211
CODEN: ORLEF7; ISSN: 1523-7060

PB American Chemical Society
DT Journal
LA English
OS CASREACT 134:178439
GI

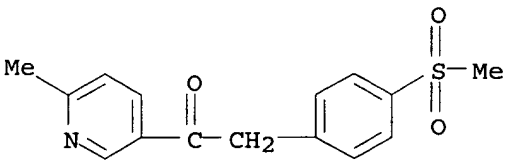


I II

AB Stabilized ketone, aldehyde, and ester enolates, generated from I (R4 = MeSO2, MeS) for example, react with vinamidinium hexafluorophosphate salts and hydroxylamine hydrochloride to give pyridine N-oxides, e.g. II (R3 = Cl, NO2), in 45-85% yields.

IT 221615-75-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyridine N-oxides by cyclization of vinamidinium salts with enolates of ketones, aldehydes, and esters)

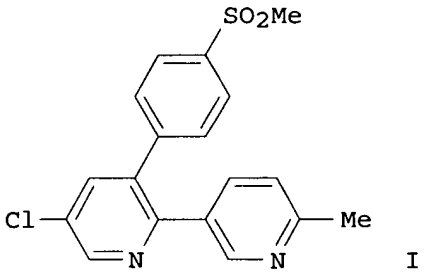
RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 12 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2000:653182 CAPLUS
DN 134:4838
TI A Practical Synthesis of a COX-2-Specific Inhibitor
AU Davies, Ian W.; Marcoux, Jean-Francois; Corley, Edward G.; Journet, Michel; Cai, Dong-Wei; Palucki, Michael; Wu, Jimmy; Larsen, Robert D.; Rossen, Kai; Pye, Philip J.; DiMichele, Lisa; Dormer, Peter; Reider, Paul J.
CS Department of Process Research, Merck Co. Inc., Rahway, NJ, 07065, USA
SO Journal of Organic Chemistry (2000), 65(25), 8415-8420
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English

OS CASREACT 134:4838
GI

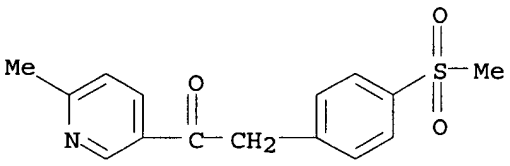



I

AB A number of synthetic strategies to the Cox-2 specific inhibitor have been described. These studies have led to the identification of a novel pyridine construction using annulation of a ketone using a vinamidinium species and ammonia in 97% assay yield. Three approaches to the synthesis of the ketone are described that allow for its preparation in large quantities in >65% overall yield from Me 6-methylnicotinate.

IT 221615-75-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of a methylsulfonylphenylbipyridine COX-2 inhibitor)

RN 221615-75-4 CAPLUS
CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)




RE.CNT 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 13 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2000:493518 CAPLUS
DN 133:104966
TI Preparation of 1-(6-methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone.
IN Armbruster, Erich; Bessard, Yves; Kuo, David; Leresche, James Edward; Proplesch, Ralf; Roduit, Jean-Paul
PA Lonza A.-G., Switz.; Merck & Co., Inc.
SO PCT Int. Appl., 19 pp.
CODEN: PIXXD2
DT Patent
LA German
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | WO 2000042014 | A2 | 20000720 | WO 2000-EP240 | 20000113 |
| | WO 2000042014 | A3 | 20001207 | | |

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

| | | | | | |
|---|---|---|---|---|---|
| | | | EP 1999-100590 | A | 19990114 |
| | | | US 1999-145996P | P | 19990729 |
| CA 2359958 | AA | 20000720 | CA 2000-2359958 | | 20000113 |
| | | | EP 1999-100590 | A | 19990114 |
| | | | US 1999-145996P | P | 19990729 |
| | | | WO 2000-EP240 | W | 20000113 |
| CA 2485739 | AA | 20000720 | CA 2000-2485739 | | 20000113 |
| | | | EP 1999-100590 | A | 19990114 |
| | | | US 1999-145996P | P | 19990729 |
| | | | CA 2000-2359958 | A3 | 20000113 |
| EP 1159270 | A2 | 20011205 | EP 2000-901555 | | 20000113 |
| EP 1159270 | B1 | 20031105 | | | |

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO

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| | | | EP 1999-100590 | A | 19990114 |
| | | | US 1999-145996P | P | 19990729 |
| | | | WO 2000-EP240 | W | 20000113 |
| JP 2003518002 | T2 | 20030603 | JP 2000-593582 | | 20000113 |
| | | | EP 1999-100590 | A | 19990114 |
| | | | US 1999-145996P | P | 19990729 |
| | | | WO 2000-EP240 | W | 20000113 |
| AT 253559 | E | 20031115 | AT 2000-901555 | | 20000113 |
| | | | EP 1999-100590 | A | 19990114 |
| | | | US 1999-145996P | P | 19990729 |
| | | | WO 2000-EP240 | W | 20000113 |
| EP 1394149 | A1 | 20040303 | EP 2003-24787 | | 20000113 |
| EP 1394149 | B1 | 20050119 | | | |

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY

| | | | | | |
|---|---|---|---|---|---|
| | | | EP 1999-100590 | A | 19990114 |
| | | | EP 2000-901555 | A3 | 20000113 |
| PT 1159270 | T | 20040331 | PT 2000-901555 | | 20000113 |
| | | | EP 1999-100590 | A | 19990114 |
| | | | US 1999-145996P | P | 19990729 |
| ES 2209807 | T3 | 20040701 | ES 2000-901555 | | 20000113 |
| | | | EP 1999-100590 | A | 19990114 |
| | | | US 1999-145996P | P | 19990729 |
| AT 287396 | E | 20050215 | AT 2003-24787 | | 20000113 |
| | | | EP 1999-100590 | A | 19990114 |
| PT 1394149 | T | 20050531 | PT 2003-24787 | | 20000113 |
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| ES 2235138 | T3 | 20050701 | ES 2003-3024787 | | 20000113 |
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| | | | WO 2000-EP240 | W | 20000113 |
| NO 2001003498 | A | 20010905 | NO 2001-3498 | | 20010713 |
| | | | EP 1999-100590 | A | 19990114 |
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| | | | WO 2000-EP240 | W | 20000113 |
| US 2005159458 | A1 | 20050721 | US 2005-29489 | | 20050106 |
| | | | EP 1999-100590 | A | 19990114 |
| | | | US 1999-145996P | P | 19990729 |

WO 2000-EP240 W 20000113
US 2003-868941 A3 20031104

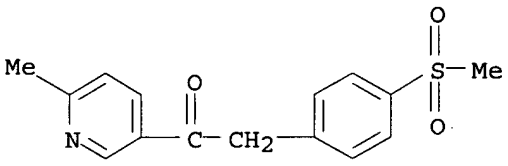
OS CASREACT 133:104966

AB 1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone (I), useful as a starting material for cyclooxygenase-2 inhibitors, was prepared Thus, N,N-diethyamino(6-methylpyridin-3-yl)acetonitrile (preparation given) and celite in PhMe were treated sequentially with aqueous NaOH, tetrabutylammonium bromide, a solution of tetrabutylammonium bromide and 4-methylsulfonylbenzyl bromide in PhMe, and tetrabutylammonium bromide followed by stirring for 6 h at 45° to give 76.4% I.

IT 221615-75-4P, 1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of 1-(6-methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



L6 ANSWER 14 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2000:443023 CAPLUS

DN 133:222553

TI Annulation of Ketones with Vinamidinium Hexafluorophosphate Salts: An Efficient Preparation of Trisubstituted Pyridines

AU Marcoux, Jean-Francois; Corley, Edward G.; Rossen, Kai; Pye, Phil; Wu, Jimmy; Robbins, Michael A.; Davies, Ian W.; Larsen, Robert D.; Reider, Paul J.

CS Department of Process Research, Merck Co. Inc., Rahway, NJ, 07065, USA

SO Organic Letters (2000), 2(15), 2339-2341
CODEN: ORLEF7; ISSN: 1523-7060

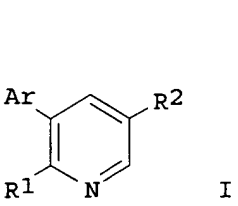
PB American Chemical Society

DT Journal

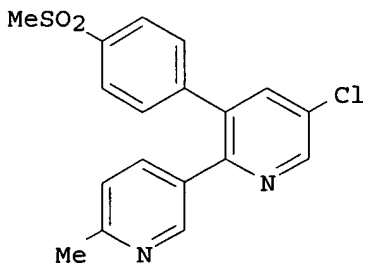
LA English

OS CASREACT 133:222553

GI



I



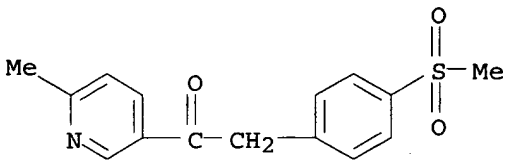
II

AB α-Aryl ketones react with vinamidinium hexafluorophosphate salts to give access to the corresponding 3-arylpyridines I (Ar = C6H4R-4, R = SO2Me, H, SMe, R1 = 6-methyl-3-pyridyl, C6H4R-4, R2 = Cl; Ar = C6H4SO2Me-4, R1 = 6-methyl-3-pyridyl, R2 = Br, I, CF3, NO2, phthalimido; Ar = C6H4F-4, R1 = Me, R2 = Cl; Ar = Ph, R1 = H, R2 = Cl). The annulation reactions proceed in good to excellent yields with vinamidinium salts containing electron-withdrawing groups at the β-position (R2). The reaction was applied to the preparation of the COX-2 specific inhibitor 5-chloro-3-(4-methylsulfonyl)phenyl-2-(2-methyl-5-pyridinyl)pyridine (II), as well as a series of analogs.

IT 221615-75-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of trisubstituted pyridines via annulation of ketones with vinamidinium hexafluorophosphate salts)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)




RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 15 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1999:708874 CAPLUS
DN 131:322542
TI Process for synthesizing arylpyridine COX-2 inhibitors
IN Corley, Edward G.; Davies, Ian W.; Larsen, Robert D.; Pye, Philip J.; Rossen, Kai
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 29 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | | DATE |
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| | | | | US 1998-82888P | P | 19980424 |
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| | | | | WO 1999-US8645 | W | 19990420 |

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| AU 759469 | | B2 | 20030417 | AU 1999-36557 | | 19990420 |
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| | | | | US 1998-85668P | P | 19980515 |
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| | | | | US 1998-85668P | P | 19980515 |
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| HR 2000000722 | | A1 | 20010630 | HR 2000-722 | | 20001024 |
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| HK 1031399 | | A1 | 20041217 | HK 2001-102195 | | 20010326 |
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| | | | | US 1998-85668P | P | 19980515 |
| | | | | WO 1999-US8645 | A | 19990420 |

OS CASREACT 131:322542; MARPAT 131:322542
GI

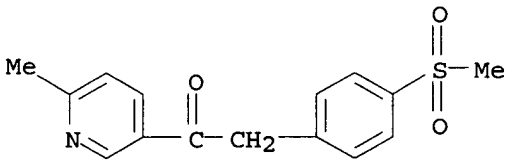
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention encompasses a process and intermediates for preparing compds. I [R, R', R'' = (un)substituted alkyl, aryl, aralkyl, halo, SOmH, SOm-alkyl, SOm-aryl, NO2, (di)(alkyl)amino, SOmNH2, SOmNH-alkyl, SOmNHCOCF3, cyano; Y = C, N; m = 0, 1, 2]. I are useful in the treatment of cyclooxygenase-2 mediated diseases (no data), i.e., as analgesics, antipyretics, and antiinflammatories. The method comprises cyclocondensation of an iminium salt II [R2-R5 = alkyl, aryl, or aralkyl; X- = suitable counterion] with an aryl ketone III in the presence of a base. The method is designed to give high yields at low temps., and with a reduced number of steps. For instance, the bipyridyl derivative IV was prepared on a 1.65-kg scale by reaction of the iminium salt V with ketone VI in THF in the presence of KOBu-tert, followed by quenching in AcOH/THF, basification with concentrated aqueous NH4OH, and refluxing. Prepns. of the salt and ketone intermediates V and VI are described, and a subset of the iminium salt intermediates II are claimed per se.

IT 221615-75-4P, 1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of arylpyridine COX-2 inhibitors by cyclocondensation of iminium salts with ketones)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)




L6 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1999:222917 CAPLUS

DN 130:252250

TI Preparation of 3-phenyl-2-(3-pyridyl)pyridines and intermediates.

IN Davies, Ian W.; Gerena, Linda; Journet, Michel; Larsen, Robert D.; Pye, Philip J.; Rossen, Kai

PA Merck & Co., Inc., USA

SO PCT Int. Appl., 42 pp.
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | WO 9915503 | A2 | 19990401 | WO 1998-US19788 | 19980922 |
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RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI,

CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

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| | | | GB 1998-6419 | A | 19980325 |
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| | | | US 1997-60680P | P | 19970925 |
| AU 9895002 | A1 | 19990412 | AU 1998-95002 | | 19980922 |
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| | | | GB 1998-6419 | A | 19980325 |
| | | | WO 1998-US19788 | W | 19980922 |
| EP 1023266 | A2 | 20000802 | EP 1998-948426 | | 19980922 |
| EP 1023266 | B1 | 20030108 | | | |

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI

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| JP 2001517654 | T2 | 20011009 | JP 2000-512812 | | 19980922 |
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| | | | WO 1998-US19788 | W | 19980922 |

OS CASREACT 130:252250; MARPAT 130:252250

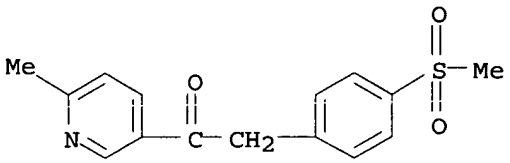
AB P-(ArCOCH2)C6H4SO2R1 (R1 = Me, NH2, NHCOCF3, NHMe; Ar = mono-, di-, or trisubstituted Ph, pyridyl, N-oxide thereof), were prepared by reaction of p-MeSC6H4CH2MgX (X = Cl, Br, F, iodo) with ArCONMe2 (Ar as above) to give p-(ArCOCH2)C6H4SMe followed by oxidation of the latter. Thus, the Grignard reagent from p-MeSC6H4CH2Cl in PhMe/THF was added to a -20° solution of 6-methylnicotinic acid N-methyl-N-methoxyamide (preparation given) in PhMe over 30 min. followed by 1 h aging to give 76% 2-methyl-5-(4-methylthiophenylacetyl)pyridine. The latter in MeOH/H2SO4 at 55° was treated with aqueous Na tungstate and then with H2O2 over 1 h to give 82.5% 2-methyl-5-(4-methylsulfonylphenylacetyl)pyridine. The latter

reacted with 3-amino-2-chloroacrolein (preparation given) to give 65% 5-chloro-2-(2-methylpyrid-5-yl)-3-(4-methylsulfonylphenyl)pyridine.

IT 221615-75-4P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 3-phenyl-2-(3-pyridyl)pyridines and intermediates)

RN 221615-75-4 CAPLUS

CN Ethanone, 1-(6-methyl-3-pyridinyl)-2-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)

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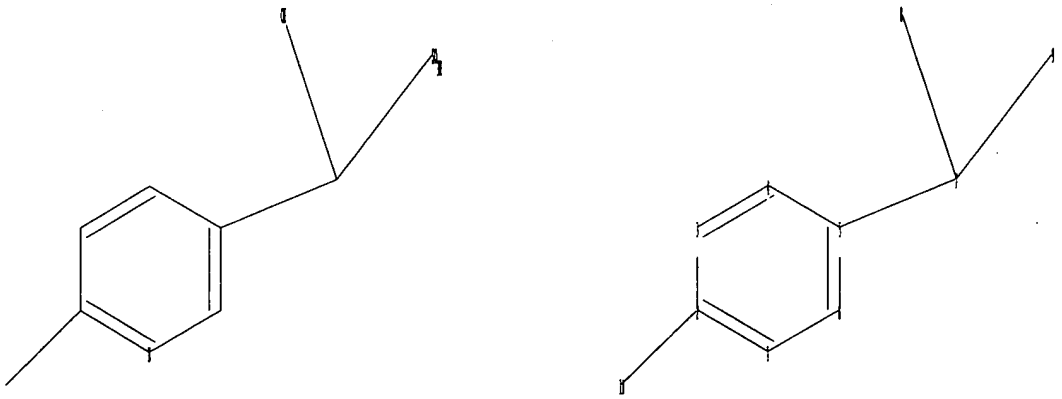

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Match level :
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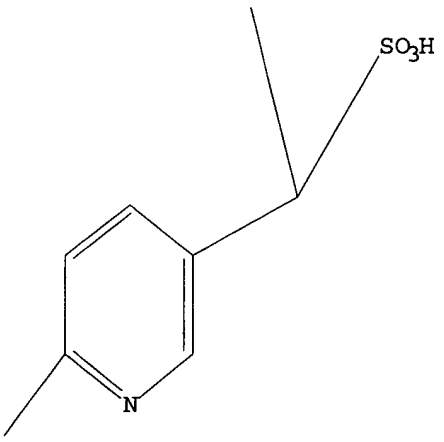


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L2 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2005 ACS on STN
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ED Entered STN: 15 Oct 2004
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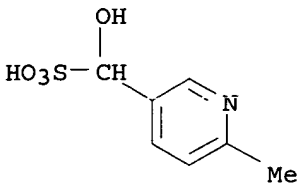
SR CA



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ED Entered STN: 04 Aug 2000
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SR CA
LC STN Files: CA, CAPLUS, USPATFULL
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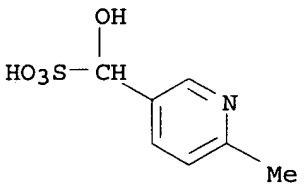

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http://www.cas.org/infopolicy.html

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L3 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2000:493518 CAPLUS
DN 133:104966
TI Preparation of 1-(6-methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone.
IN Armbruster, Erich; Bessard, Yves; Kuo, David; Leresche, James Edward; Proplesch, Ralf; Roduit, Jean-Paul
PA Lonza A.-G., Switz.; Merck & Co., Inc.
SO PCT Int. Appl., 19 pp.
CODEN: PIXXD2
DT Patent
LA German
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | | DATE |
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| PI | WO 2000042014 | A2 | 20000720 | WO 2000-EP240 | | 20000113 |
| | WO 2000042014 | A3 | 20001207 | | | |
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| | RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | | |
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| | | | | US 1999-145996P | P | 19990729 |
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| EP 1159270 | | A2 | 20011205 | EP 2000-901555 | | 20000113 |
| EP 1159270 | | B1 | 20031105 | | | |
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| | | | | WO 2000-EP240 | W | 20000113 |
| JP 2003518002 | | T2 | 20030603 | JP 2000-593582 | | 20000113 |
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| AT 253559 | | E | 20031115 | AT 2000-901555 | | 20000113 |
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| | | | | WO 2000-EP240 | W | 20000113 |
| EP 1394149 | | A1 | 20040303 | EP 2003-24787 | | 20000113 |
| EP 1394149 | | B1 | 20050119 | | | |
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| NO 2001003498 | | A | 20010905 | NO 2001-3498 | | 20010713 |
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| US 2005159458 | | A1 | 20050721 | US 2005-29489 | | 20050106 |
| | | | | EP 1999-100590 | A | 19990114 |
| | | | | US 1999-145996P | P | 19990729 |
| | | | | WO 2000-EP240 | W | 20000113 |
| | | | | US 2003-868941 | A3 | 20031104 |

OS CASREACT 133:104966

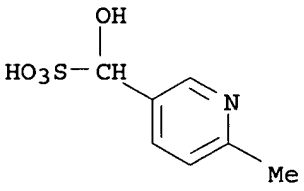
AB 1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone (I), useful as a starting material for cyclooxygenase-2 inhibitors, was prepared Thus, N,N-diethyamino(6-methylpyridin-3-yl)acetonitrile (preparation given) and celite in PhMe were treated sequentially with aqueous NaOH, tetrabutylammonium bromide, a solution of tetrabutylammonium bromide and 4-methylsulfonylbenzyl bromide in PhMe, and tetrabutylammonium bromide followed by stirring for 6 h at 45° to give 76.4% I.

IT 283167-58-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 1-(6-methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone)

RN 283167-58-8 CAPLUS

CN 3-Pyridinemethanesulfonic acid, α-hydroxy-6-methyl-, monosodium salt

(9CI) (CA INDEX NAME)



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FULL ESTIMATED COST                                 7.19     173.27

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)    SINCE FILE      TOTAL
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